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Adiabatic Perturbation Theory in Quantum Dynamics

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1 Introduction

Separation of scales plays a fundamental role in the understanding of the dynamical behavior of complex systems in physics and other natural sciences. It is often possible to derive simple laws for certain slow variables from the underlying fast dynamics whenever the scales are well separated. Clearly the manifestations of this basic idea and the precise meaning of slow and fast may differ widely. A spinning top may serve as a simple example for the kind of situation we shall consider. While it is spinning at a high frequency, the rotation axis is usually precessing much slower. The orientation of the rotation axis is thus the slow degree of freedom, while the angle of rotation with respect to the axis is the fast degree of freedom. The earth is an example of a top where these scales are well separated. It turns once a day, but the frequency of precession is about once in 25700 years.

In this monograph we consider quantum mechanical systems which display such a separation of scales. The prototypic example are molecules, i.e. systems consisting of two types of particles with very different masses. Electrons are lighter than nuclei by at least a factor of $2 \cdot 10^3$, depending on the type of nucleus. Therefore, assuming equal distribution of kinetic energies inside a molecule, the electrons are moving at least 50 times faster than the nuclei. The effective dynamics for the slow degrees of freedom, i.e. for the nuclei, is known as the Born-Oppenheimer approximation and it is of extraordinary importance for understanding molecular dynamics. Roughly speaking, in the Born-Oppenheimer approximation the nuclei evolve in an effective potential generated by one energy level of the electrons, while the state of the electrons instantaneously adjusts to an eigenstate corresponding to the momentary configuration of the nuclei. The phenomenon that fast degrees of freedom become slaved by slow degrees of freedom which in turn evolve autonomously is called adiabatic decoupling.

We will find that there is a variety of physical systems which have the same mathematical structure as molecular dynamics and for which similar mathematical methods can be applied in order to derive effective equations of motion for the slow degrees of freedom. The unifying characteristic, which is reflected in the common mathematical structure described below, is that the fast scale is always also the quantum mechanical time scale defined through Planck's constant $\hbar$ and the relevant energies. The slow scale is "slow" with

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respect to the fast quantum scale. However, the underlying physical mechanisms responsible for scale separation and the qualitative features of the arising effective dynamics may differ widely.

The abstract mathematical question we are led to when considering the problem of adiabatic decoupling in quantum dynamics, is the singular limit $\varepsilon \to 0$ in Schrödinger's equation

$$\mathrm{i}\,\varepsilon \frac{\partial}{\partial t}\,\psi^{\varepsilon}(t,x) = H(x, -\mathrm{i}\varepsilon\nabla_x)\,\psi^{\varepsilon}(t,x) \tag{1.1}$$

with a special type of Hamiltonian H. For fixed time $t \in \mathbb{R}$ the wave function $\psi(t,\cdot)$ of the system is an element of the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathcal{H}_{\mathrm{f}}$, where $L^2(\mathbb{R}^d)$ is the state space for the slow degrees of freedom and $\mathcal{H}_{\mathrm{f}}$ is the state space for the fast degrees of freedom. The Hamiltonian $H(x, -\mathrm{i}\varepsilon\nabla_x)$ is a linear operator acting on this Hilbert space and generates the time-evolution of states in $\mathcal{H}$. As indicated by the notation, the Hamiltonian is a pseudodifferential operator. More precisely, $H(x, -\mathrm{i}\varepsilon\nabla_x)$ is the Weyl quantization of a function $H : \mathbb{R}^{2d} \to \mathcal{L}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}})$ with values in the self-adjoint operators on $\mathcal{H}_{\mathrm{f}}$. As needs to be explained, the parameter $0 < \varepsilon \ll 1$ controls the separation of scales: the smaller ε the better is the slow time scale separated from the fixed fast time scale.

Equation (1.1) provides a complete description of the quantum dynamics of the entire system. However, in many interesting situations the complexity of the full system makes a numerical treatment of (1.1) impossible, today and in the foreseeable future. Even a qualitative understanding of the dynamics can often not be based on the full equations of motion (1.1) alone. It is therefore of major interest to find simpler effective equations of motion that yield at least approximate solutions to (1.1) whenever ε is sufficiently small.

This monograph reviews and extends a quite recent approach to adiabatic perturbation theory in quantum dynamics. Roughly speaking the goal of this approach is to find asymptotic solutions to the initial value problem (1.1) as solutions of an effective Schrödinger equation for the slow degrees of freedom alone. It turns out that in many situations this effective Schrödinger equation is not only simpler than (1.1), but can be further analyzed using methods of semiclassical approximation. Indeed, in other approaches the limit $\varepsilon \to 0$ in (1.1) is understood as a partial semiclassical limit for certain degrees of freedom only, namely for the slow degrees of freedom. We believe that one main insight of our approach is the clear separation of the adiabatic limit from the semiclassical limit. Indeed, it turns out that adiabatic decoupling is a necessary condition for semiclassical behavior of the slow degrees of freedom. Semiclassical behavior is, however, not a necessary consequence of adiabatic decoupling. This is exemplified by the double slit experiment for electrons as Dirac particles. While the coupling to the positrons can be neglected in very good approximation, because of interference effects the electronic part behaves by no means semiclassical.

A closely related feature of our approach – worth stressing – is the clear emphasis on effective equations of motion throughout all stages of the construction. As opposed to the direct construction of approximate solutions to (1.1) based on the WKB Ansatz or on semiclassical wave packets, this has two advantages. The obvious point is that effective equations of motion allow one to prove results for general states, not only for those within some class of nice Ansatz functions. More important is, however, that the higher order corrections in the effective equations of motion allow for a straightforward physical interpretation. In contrast it is not obvious how to gain the same physical picture from the higher order corrections to the special solutions. This last point is illustrated e.g. by the derivation of corrections to the semiclassical model of solid state physics based on coherent states in [SuNi]. There it is not obvious how to conclude from the corrections to the solution on the corrections to the dynamical equations. As a consequence in [SuNi] one ε-dependent force term was missed in the semiclassical equations of motion, cf. Sections 5.1 and 5.3.

Adiabatic perturbation theory constitutes an example where techniques of mathematical physics yield more than just a rigorous confirmation of results well known to physicists. To the contrary, the results provide new physical insights into adiabatic problems and yield novel effective equations, as witnessed, for example, by the corrections to the semiclassical model of solid state physics as derived in Section 5.3 or by the non-perturbative formula for the g-factor in non-relativistic QED as presented in [PST$_2$]. However, the physics literature on adiabatic problems is extensive and we mention at this point the work of Blount [Bl$_1$, Bl$_2$, Bl$_3$] and of Littlejohn et. al. [LiFl$_1$, LiFl$_2$, LiWe$_1$, LiWe$_2$], since their ideas are in part quite close to ours. A very recent survey of adiabatic problems in physics is the book of Bohm, Mostafazadeh, Koizumi, Niu and Zwanziger [BMKNZ].

Apart from this introductory chapter the book at hand contains three main parts. First order adiabatic theory for a certain type of problems, namely for perturbations of fibered Hamiltonians, is discussed and applied in Chapter 2. Here and in the following "order" refers to the order of approximation with respect to the parameter ε. The mathematical tools used in Chapter 2 are those contained in any standard course dealing with unbounded self-adjoint operators on Hilbert spaces, e.g. [ReSi$_1$]. The proofs are motivated by strategies developed in the context of the time-adiabatic theorem of quantum mechanics by Kato [Ka$_2$], Nenciu [Nen$_4$] and Avron, Seiler and Yaffe [ASY$_1$]. Several results presented in Chapter 2 emerged from joint work of the author with H. Spohn [SpTe, TeSp].

In Chapter 3 we attack the general problem in the form of Equation (1.1) on an abstract level and develop a theory, which allows for approximations to arbitrary order. Chapter 4 and Chapter 5 contain applications and extensions of this general scheme, which we term *adiabatic perturbation theory*. As can be seen already from the formulation of the problem in (1.1),

the main mathematical tool of Chapters 3–5 are pseudodifferential operators with operator-valued symbols. For the convenience of the reader, we collect in Appendix A the necessary definitions and results and give references to the literature. In our context pseudodifferential operators with operator-valued symbols were first considered by Balazard-Konlein [Ba] and applied many times to related problems, most prominently by Helffer and Sjöstrand [HeSj], by Klein, Martinez, Seiler and Wang [KMSW] and by Gérard, Martinez and Sjöstrand [GMS]. While more detailed references are given within the text, we mention that the basal construction of Section 3.1 appeared already several times in the literature. Special cases were considered by Emmrich and Weinstein [EmWe], Brummelhuis and Nourrigat [BrNo] and by Martinez and Sordoni [MaSo], while the general case is due to Nenciu and Sordoni [NeSo]. Many of the original results presented in Chapters 3–5 stem from a collaboration of the author with G. Panati and H. Spohn [PST_1, PST_2, PST_3].

The first five chapters deal with adiabatic decoupling in the presence of a gap in the spectrum of the symbol $H(q,p) \in \mathcal{L}_{\mathrm{sa}}(\mathcal{H}_{\mathrm{f}})$ of the Hamiltonian. Chapter 6 is concerned with adiabatic theory without spectral gap, which was started, in a general setting, only recently by Avron and Elgart [AvEl_1] and by Bornemann [Bor]. Most results presented in Chapter 6 appeared in [Te_1, Te_2].

The reader might know that adiabatic theory is well developed also for classical mechanics, see e.g. [LoMe]. Although a careful comparison of the quantum mechanical results with those of classical adiabatic theory would seem an interesting enterprize, this is beyond the scope of this monograph. We will remain entirely in the framework of quantum mechanics with the exception of Section 2.4, where some aspects of such a comparison are discussed in a special example.

Since it requires considerable preparation to enter into more details, we postpone a detailed outline and discussion of the contents of this book to the end of the introductory chapter.

In order to get a feeling for adiabatic problems in quantum mechanics and for the concepts involved in their solution, we recall in Section 1.1 the "adiabatic theorem of quantum mechanics" which can be found in many textbooks on theoretical physics. For reasons that become clear later on we shall refer to it as the time-adiabatic theorem. Afterwards in Section 1.2 two examples from physics are discussed, where instead of a time-adiabatic theorem a space-adiabatic theorem can be formulated. While molecular dynamics and the Born-Oppenheimer approximation motivate the investigations of Chapter 2, adiabatic decoupling for the Dirac equation with slowly varying external fields will lead us directly to the general formulation of the problem as in (1.1).

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1.1 The time-adiabatic theorem of quantum mechanics

The purpose of this section is to introduce a number of concepts that will accompany us throughout this monograph. This is done in the context of the time-adiabatic theorem, which is the simplest and at the same time the prototype of adiabatic theorems in quantum mechanics. Indeed, the prefix *time* is often omitted and the time-adiabatic theorem is what one usually means by *the* adiabatic theorem. As a consequence, most of the mathematical investigations were concerned with the time-adiabatic setting and a deep and general understanding has been achieved since the first formulation of the idea by Ehrenfest [Eh] in 1916 and the pioneering work by Born and Fock [BoFo] from 1928.

However, since the present section is mostly concerned with a simple outline of basic concepts, we will *not* aim at the broadest generality. To the contrary, we will avoid technicalities as much as possible for the moment and postpone bibliographical remarks to the end of this section and to Chapter 2. Our presentation of the time-adiabatic theorem is neither the most concise one nor the standard one, but allows for the most direct generalization to the space-adiabatic setting.

The time-adiabatic theorem is concerned with quantum systems described by a Hamiltonian explicitly but slowly depending on time. The explicit time-dependence of the Hamiltonian stems in some applications from a time-dependence of external parameters such as an electric field, which is slowly turned on. However, often the slowly varying parameters come from an idealization of the coupling to another quantum system. The idealization consists in prescribing the time-dependent configurations of the other system in the Hamiltonian of the full quantum system. It is the content of space-adiabatic theory to understand adiabatic decoupling without relying on this idealization, as to be explained in detail in the next section.

Let $H(s)$, $s \in \mathbb{R}$, be a family of bounded self-adjoint operators on some Hilbert space $\mathcal{H}$. One is interested in the solution of the initial value problem

$$\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}s}\,\widetilde{U}^{\varepsilon}(s,s_0) = H(\varepsilon s)\,\widetilde{U}^{\varepsilon}(s,s_0)\,, \quad \widetilde{U}^{\varepsilon}(s_0,s_0) = \mathbf{1}_{\mathcal{H}}\,. \tag{1.2}$$

The small parameter ε controls the time-scale on which $H(\varepsilon s)$ varies and is discussed below. If the map $s \mapsto H(s)$ is strongly continuous, then it is easy to construct the unitary propagator $\widetilde{U}^{\varepsilon}(s,s_0)$ solving (1.2) by means of a Dyson expansion, cf. [ReSi$_2$].

Definition 1.1. *A unitary propagator is a jointly strongly continuous family $U(s,t)$ of unitary operators satisfying*

(i) $U(s,r)\,U(r,t) = U(s,t)$ *for all* $s,r,t \in \mathbb{R}$
(ii) $U(s,s) = \mathbf{1}_{\mathcal{H}}$ *for all* $s \in \mathbb{R}$.

Clearly, if $\widetilde{U}^\varepsilon(s, s_0)$ solves (1.2), then $\psi(s) = \widetilde{U}^\varepsilon(s, s_0)\,\psi_0$ solves the Schrödinger equation

$$\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}s}\,\psi(s) = H(\varepsilon s)\,\psi(s) \quad \text{with initial condition} \quad \psi(s_0) = \psi_0\,. \tag{1.3}$$

The parameter $\varepsilon > 0$ in (1.2) resp. (1.3) is the adiabatic parameter and controls the separation of time-scales. Note that the smaller ε, the slower is the variation of $H(\varepsilon s)$ on the *a priori* fixed fast or microscopic time-scale. The time-scale $t = \varepsilon s$ on which H varies is called the slow or macroscopic time-scale. Throughout this monograph we adopt the following conventions.

– Times measured in *fast or microscopic* units are denoted by the letter s.
– Times measured in *slow or macroscopic* units are denoted by the letter t.
– The fast and the slow time-scales are related as

$$t = \varepsilon s$$

through the scale parameter $0 < \varepsilon \ll 1$.

The notions macro- and microscopic might appear somewhat out of place here. At the moment we use them synonymously for slow and fast. However, in many applications the appearance of different time scales is closely related to the existence of different spatial scales. Then the use of micro- and macroscopic becomes more natural.

On the slow time-scale (1.2) reads

$$\mathrm{i}\,\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\,U^\varepsilon(t, t_0) = H(t)\,U^\varepsilon(t, t_0)\,, \quad U^\varepsilon(t_0, t_0) = \mathbf{1}\,, \tag{1.4}$$

where $U^\varepsilon(t, t_0) = \widetilde{U}^\varepsilon(t/\varepsilon, t_0/\varepsilon)$. Since H varies on the slow time-scale, one expects nontrivial effects to happen on this time-scale and thus the object of the following investigations are solutions to (1.4) at finite macroscopic times.

The content of the time-adiabatic theorem is that $U^\varepsilon(t, t_0)$ approximately transports the time-dependent spectral subspaces of $H(t)$ which vary sufficiently smoothly as t changes. In the classical result one considers spectral subspaces associated with parts of the spectrum which are separated by a gap from the remainder. More precisely, assume that the spectrum $\sigma(t)$ of $H(t)$ contains a subset $\sigma_*(t) \subset \sigma(t)$, such that there are two bounded continuous functions $f_\pm \in C_\mathrm{b}(\mathbb{R}, \mathbb{R})$ defining an interval $I(t) = [f_-(t), f_+(t)]$ with

$$\sigma_*(t) \subset I(t) \quad \text{and} \quad \inf_{t\in\mathbb{R}} \mathrm{dist}\big(I(t), \sigma(t) \setminus \sigma_*(t)\big) =: g > 0\,. \tag{1.5}$$

The previous definition of "separated by a gap" might look slightly complicated, but encodes exactly the simple picture displayed in Figure 1.1.

Let $P_*(t)$ be the spectral projection of $H(t)$ on $\sigma_*(t)$, then, assuming sufficient regularity for $H(t)$, the **time-adiabatic theorem of quantum**

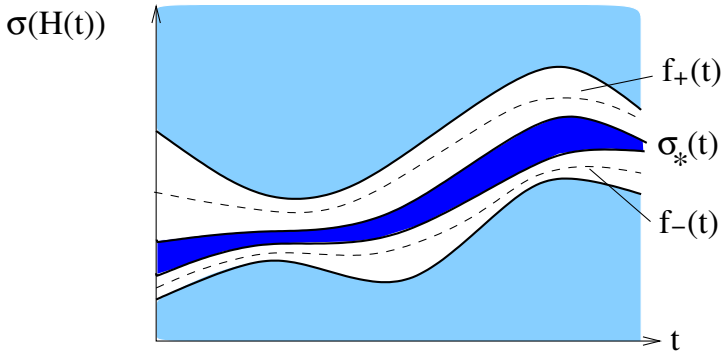

Fig. 1.1. Spectrum which is locally isolated by a gap.

mechanics in its simplest form states that there is a constant $C < \infty$ such that

$$\left\| \left(\mathbf{1} - P_*(t)\right) U^\varepsilon(t, t_0)\, P_*(t_0) \right\|_{\mathcal{L}(\mathcal{H})} \leq C\, \varepsilon\, (1 + |t - t_0|)\,. \tag{1.6}$$

Physically speaking, if a system is initially in the state $\psi_0 \in P_*(t_0)\mathcal{H}$, then the state of the system at later times $\psi(t)$ given through the solution of (1.3) stays in the subspace $P_*(t)\mathcal{H}$ up to an error of order $\mathcal{O}(\varepsilon(1 + |t - t_0|)\|\psi_0\|)$. The analogous assertion holds true if one starts in the orthogonal complement of $P_*(t_0)\mathcal{H}$.

The mechanism that spectral subspaces which depend in some sense slowly on some parameter are approximately invariant under the quantum mechanical time-evolution is called **adiabatic decoupling**.

While the time-adiabatic theorem is often stated in the form (1.6), its proof as going back to Kato [Ka$_2$] yields actually a stronger statement than (1.6). Let

$$H_{\mathrm{a}}(t) = H(t) - \mathrm{i}\,\varepsilon P_*(t)\,\dot{P}_*(t) - \mathrm{i}\,\varepsilon P_*^\perp(t)\,\dot{P}_*^\perp(t) \tag{1.7}$$

be the *adiabatic Hamiltonian*, where $P_*^\perp(t) = \mathbf{1} - P_*(t)$, and let $U_{\mathrm{a}}^\varepsilon(t, t_0)$ be the *adiabatic propagator* given as the solution of

$$\mathrm{i}\,\varepsilon \frac{\mathrm{d}}{\mathrm{d}t}\, U_{\mathrm{a}}^\varepsilon(t, t_0) = H_{\mathrm{a}}(t)\, U_{\mathrm{a}}^\varepsilon(t, t_0)\,, \quad U_{\mathrm{a}}^\varepsilon(t_0, t_0) = \mathbf{1}\,. \tag{1.8}$$

As to be shown, the adiabatic propagator is constructed such that it intertwines the spectral subspaces $P_*(t)$ at different times *exactly*, i.e.

$$P_*(t)\, U_{\mathrm{a}}^\varepsilon(t, t_0) = U_{\mathrm{a}}^\varepsilon(t, t_0)\, P_*(t_0) \quad \text{for all } t, t_0 \in \mathbb{R}\,. \tag{1.9}$$

We are now in a position to state the **strong version of the time-adiabatic theorem**.

Theorem 1.2. *Let $H(\cdot) \in C^2_{\rm b}(\mathbb{R}, \mathcal{L}_{\rm sa}(\mathcal{H}))$ and let $\sigma_*(t) \subset \sigma(H(t))$ satisfy the gap condition (1.5). Then $P_* \in C^2_{\rm b}(\mathbb{R}, \mathcal{L}(\mathcal{H}))$ and there is a constant $C < \infty$ such that for all $t, t_0 \in \mathbb{R}$*

$$\| U^\varepsilon(t, t_0) - U^\varepsilon_{\rm a}(t, t_0)\| \leq C\, \varepsilon\, (1 + |t - t_0|)\,. \tag{1.10}$$

By virtue of (1.9), (1.10) implies (1.6). Statement (1.10) is stronger than (1.6) since it yields not only approximate invariance of the spectral subspace, but gives also information about the *effective time-evolution inside the decoupled subspace*, a feature that will occupy us throughout this monograph.

While the detailed proof of Theorem 1.2 is postponed to the beginning of Chapter 2, let us shortly explain the mechanism. A straightforward calculation shows that the difference $U^\varepsilon(t, t_0) - U^\varepsilon_{\rm a}(t, t_0)$ can be written as an integral

$$U^\varepsilon(t, t_0) - U^\varepsilon_{\rm a}(t, t_0) = \int_{t_0}^t {\rm d}t'\, A^\varepsilon(t')\,. \tag{1.11}$$

However, since the quantity $A^\varepsilon(t')$ is $\mathcal{O}(1)$, a naive estimate would give that $U^\varepsilon(t, t_0) - U^\varepsilon_{\rm a}(t, t_0) = \mathcal{O}(1)|t - t_0|$. The key observation for getting (1.10) is that $A^\varepsilon(t')$ is oscillating at a frequency proportional to $1/\varepsilon$. Hence a careful estimate of the right hand side of (1.11) yields (1.10) as in the simple example

$$\int_{t_0}^t {\rm d}t'\, {\rm e}^{{\rm i}t'/\varepsilon} = -{\rm i}\varepsilon \left({\rm e}^{{\rm i}t_0/\varepsilon} - {\rm e}^{{\rm i}t/\varepsilon} \right) = \mathcal{O}(\varepsilon)\,.$$

The spectral gap condition enters in two ways. It is not only crucial in order to show that A is oscillating with a frequency uniformly larger than a constant times $1/\varepsilon$, but it is also essential to conclude the regularity of $P_*(\cdot)$ from the regularity of $H(\cdot)$.

It remains to check (1.9). Naively one could think that $U^\varepsilon(t, t_0)$ itself satisfies (1.9), or equivalently that

$$U^\varepsilon(t_0, t)\, P_*(t)\, U^\varepsilon(t, t_0) = P_*(t_0) \qquad \text{(NOT TRUE)}\,. \tag{1.12}$$

After all, $P_*(t)$ are spectral projections of $H(t)$ and thus $[H(t), P_*(t)] = 0$. However, taking a derivative with respect to t of the left hand side in (1.12) yields

$$\begin{aligned} &\frac{\rm d}{{\rm d}t}\big(U^\varepsilon(t_0, t)\, P_*(t)\, U^\varepsilon(t, t_0)\big) = \qquad\qquad (1.13)\\ &\quad = -\frac{\rm i}{\varepsilon}\, U^\varepsilon(t_0, t)\, [H(t), P_*(t)]\, U^\varepsilon(t, t_0) + U^\varepsilon(t_0, t)\, \dot P_*(t)\, U^\varepsilon(t, t_0) = \\ &\quad = U^\varepsilon(t_0, t)\, \dot P_*(t)\, U^\varepsilon(t, t_0) \neq 0 \end{aligned}$$

and thus (1.12) cannot hold for $t \neq t_0$. But from (1.13) we easily read off what to do. In order to define a propagator satisfying (1.12) one has to add an operator $M(t)$ to the generator $H(t)$ such that

$$\dot{P}_*(t) = \frac{\mathrm{i}}{\varepsilon}[M(t), P_*(t)]\,. \tag{1.14}$$

Hence we are left to check that the choice of $M(t)$ made in (1.7) satisfies (1.14). To this end observe that

$$\dot{P}_*(t) = \frac{\mathrm{d}}{\mathrm{d}t}(P_*(t))^2 = \dot{P}_*(t)P_*(t) + P_*(t)\dot{P}_*(t)$$

implies

$$\dot{P}_*(t) = P_*^{\perp}(t)\,\dot{P}_*(t)\,P_*(t) + P_*(t)\,\dot{P}_*(t)\,P_*^{\perp}(t)\,. \tag{1.15}$$

Although quite obvious, the fact that the derivative of a family of orthogonal projections is block diagonal with respect to the block decomposition it induces, turns out to be crucial for all what follows. With (1.15) we find that

$$H_{\mathrm{a}}(t) = H(t) + \mathrm{i}\,\varepsilon\,[\dot{P}_*(t), P_*(t)] \tag{1.16}$$

and that (1.14) is satisfied for $M(t) = \mathrm{i}\,\varepsilon\,[\dot{P}_*(t), P_*(t)]$,

$$\dot{P}_*(t) = \big[\,[\dot{P}_*(t), P_*(t)],\, P_*(t)\,\big] = -\frac{\mathrm{i}}{\varepsilon}\,\big[\,\mathrm{i}\,\varepsilon\,[\dot{P}_*(t), P_*(t)], P_*(t)\big]\,.$$

Remark 1.3. In some applications one has more than two parts of the spectrum which are mutually separated by a gap. As observed by Nenciu [Nen$_4$], the generalization to this case is straightforward and the adiabatic Hamiltonian would take the form

$$H_{\mathrm{a}}(t) = H(t) - \mathrm{i}\,\varepsilon \sum_{j=1}^{N} P_j(t)\,\dot{P}_j(t)\,,$$

where $P_j(t)$ is the spectral projection on the j^{th} separated component of the spectrum. ♢

Effective dynamics

In many situations one is interested only in the dynamics inside the subspaces $P_*(t)\mathcal{H}$, which might be of particular interest for physical reasons or just be selected by the initial condition. If, for example, $\sigma_*(t) = \{E(t)\}$ is a single eigenvalue of finite multiplicity ℓ, then $P_*(t)\mathcal{H} \cong \mathbb{C}^\ell$ for all $t \in \mathbb{R}$ and the adiabatic evolution $U_{\mathrm{a}}^{\varepsilon}(t, t_0)$ restricted to $P_*(t)\mathcal{H}$ can be mapped unitarily to an evolution on the time-independent space $\mathbb{C}^\ell$. The effective dynamics on the **reference space** $\mathbb{C}^\ell$ takes an especially simple form.

To see this let $\{\varphi_\alpha(t)\}_{\alpha=1}^{\ell}$ be an orthonormal basis of $P_*(t)\mathcal{H}$ such that $\varphi_\alpha(t) \in C_{\mathrm{b}}^1(\mathbb{R}, \mathcal{H})$ for all α. Such a basis always exists under the conditions of Theorem 1.2, take for example $\{U_{\mathrm{a}}^{\varepsilon=1}(t, t_0)\,\varphi_\alpha(t_0)\}_{\alpha=1}^{\ell}$ for some fixed orthonormal basis $\{\varphi_\alpha(t_0)\}_{\alpha=1}^{\ell}$ of $P_*(t_0)\mathcal{H}$. Let $\{\chi_\alpha\}_{\alpha=1}^{\ell}$ be an orthonormal basis of $\mathbb{C}^\ell$ and define the time-dependent unitary $\mathcal{U}(t) : P_*(t)\mathcal{H} \to \mathbb{C}^\ell$ as

$$\mathcal{U}(t) = \sum_{\alpha=1}^{\ell} |\chi_\alpha\rangle\langle\varphi_\alpha(t)| \,. \tag{1.17}$$

We use the physicist's notation $|\chi\rangle\langle\varphi|\,\psi := \langle\varphi,\psi\rangle_{\mathcal{H}}\,\chi$. Then

$$U^\varepsilon_{\text{eff}}(t,t_0) = \mathcal{U}(t)\, U^\varepsilon_{\text{a}}(t,t_0)\, \mathcal{U}^*(t_0) \tag{1.18}$$

defines a unitary propagator on the reference space $\mathbb{C}^\ell$. As we will show, it can be obtained as the solution of the Schrödinger equation

$$\mathrm{i}\,\varepsilon \frac{\mathrm{d}}{\mathrm{d}t}\, U^\varepsilon_{\text{eff}}(t,t_0) = H^\varepsilon_{\text{eff}}(t)\, U^\varepsilon_{\text{eff}}(t,t_0)\,, \quad U^\varepsilon_{\text{eff}}(t_0,t_0) = \mathbf{1}_{\mathbb{C}^\ell} \tag{1.19}$$

with effective Hamiltonian

$$H^\varepsilon_{\text{eff}}(t)_{\alpha\beta} = E(t)\,\delta_{\alpha\beta} - \mathrm{i}\,\varepsilon\,\langle\varphi_\alpha(t), \dot\varphi_\beta(t)\rangle_{\mathcal{H}}\,, \tag{1.20}$$

where $\alpha,\beta = 1,\ldots,\ell$ are matrix-indices with respect to the basis $\{\chi_\alpha\}_{\alpha=1}^{\ell}$.

Theorem 1.4. *Assume the conditions of Theorem 1.2 and, in addition, that $\sigma_*(t) = \{E(t)\}$ is a single eigenvalue of finite multiplicity ℓ. Then there is a constant $C < \infty$ such that the solution of (1.19) satisfies*

$$\left\| \left(U^\varepsilon(t,t_0) - \mathcal{U}^*(t)\, U^\varepsilon_{\text{eff}}(t,t_0)\,\mathcal{U}(t_0)\right) P_*(t_0) \right\| \leq C\,\varepsilon\,(1+|t-t_0|)\,. \tag{1.21}$$

While Theorem 1.4 is mathematically not deep at all, conceptually it is a very important step. The observation that the subspaces $P_*(t)\mathcal{H}$ are not only adiabatically decoupled from the remainder of the Hilbert space, but that the dynamics inside of them can be formulated in terms of a much simpler Schrödinger equation as (1.19), turns out to produce many interesting results. In Section 1.2 of the introduction, we obtain, e.g., the famous Thomas-BMT equation for the spin-dynamics of a relativistic spin-$\frac{1}{2}$ particle from (1.20) and (1.21).

Proof (of Theorem 1.4). Knowing already that (1.10) holds, all we need to show is that $U^\varepsilon_{\text{eff}}(t,t_0)$ defined through (1.18) is indeed given as the unique solution of (1.19). To this end we differentiate (1.18) with respect to t and find

$$\begin{aligned} \mathrm{i}\,\varepsilon \frac{\mathrm{d}}{\mathrm{d}t}\, U^\varepsilon_{\text{eff}}(t,t_0) &= \mathcal{U}(t)\, H^\varepsilon_{\text{a}}(t)\, U^\varepsilon_{\text{a}}(t,t_0)\,\mathcal{U}^*(t_0) + \mathrm{i}\,\varepsilon\dot{\mathcal{U}}(t)\, U^\varepsilon_{\text{a}}(t,t_0)\,\mathcal{U}^*(t_0) \\ &= \left(\mathcal{U}(t)\, H^\varepsilon_{\text{a}}(t)\,\mathcal{U}^*(t) + \mathrm{i}\,\varepsilon\dot{\mathcal{U}}(t)\,\mathcal{U}^*(t)\right) U^\varepsilon_{\text{eff}}(t,t_0)\,. \end{aligned} \tag{1.22}$$

Hence $U^\varepsilon_{\text{eff}}(t,t_0)$ satisfies (1.19) with

$$\begin{aligned} H^\varepsilon_{\text{eff}}(t) &= \mathcal{U}(t)\, H^\varepsilon_{\text{a}}(t)\,\mathcal{U}^*(t) + \mathrm{i}\,\varepsilon\dot{\mathcal{U}}(t)\,\mathcal{U}^*(t) \\ &= \mathcal{U}(t)\, H^\varepsilon(t)\,\mathcal{U}^*(t) + \mathrm{i}\,\varepsilon\dot{\mathcal{U}}(t)\,\mathcal{U}^*(t) \end{aligned}$$

and a straightforward calculation yields the matrix-representation (1.20). □

Generalizations

In summary Theorem 1.2 and Theorem 1.4 contain what we will call **first order time-adiabatic theory with gap condition**. The terminology suggests already that there are several ways of generalizing this theory.

(i) Adiabatic theorems with higher order error estimates and **higher order** asymptotic expansions in the adiabatic parameter ε.
(ii) Adiabatic theorems **without a gap** condition.
(iii) **Space-adiabatic** theorems, where the slow variation is of dynamical origin and not put in "by hand" through a Hamiltonian depending slowly on time.

Time-adiabatic theorems with improved error estimates were extensively explored in the literature and we will sketch the type of results available shortly. Time-adiabatic theorems without gap condition are only quite recent and their understanding is much less developed. We will comment no further on how to remove the gap condition in this section, but refer to Chapter 6, which is devoted to adiabatic decoupling without spectral gap. Space-adiabatic theory in the general form to be presented in this monograph is quite recent and will be motivated and set up in Section 1.2.

We close this introductory section on the time-adiabatic theorem with some remarks on higher order estimates. Going back to the beginning of this section, the error estimate in (1.6) is undoubtedly correct, but it really begs the question, since the nature of $\mathcal{O}(\varepsilon)$ is left unspecified. There are basically two alternatives.

(a) There is a piece of the wave function $\psi(t) = U^\varepsilon(t, t_0)\psi(t_0)$ of order ε that "leaks out" into the complement of $P_*(t)\mathcal{H}$. More precisely (1.6) could be optimal in the sense that the error really grows like $\varepsilon|t - t_0|$.
(b) The state $\psi(t)$ remains for much longer times in a subspace $P_*^\varepsilon(t)\mathcal{H}$ which is only slightly tilted with respect to $P_*(t)\mathcal{H}$, in the sense that $\|P_*(t) - P_*^\varepsilon(t)\| = \mathcal{O}(\varepsilon)$.

As first recognized by Lenard [Le], and on a more refined level by Garrido [Ga], Avron, Seiler and Yaffe [ASY$_1$], Nenciu [Nen$_1$] and by Joye, Kunz and Pfister [JKP], it is the latter option which is realized by the solution to (1.4). If $H(\cdot) \in C_{\mathrm{b}}^\infty(\mathbb{R}, \mathcal{L}_{\mathrm{sa}}(\mathcal{H}))$ then there is an iterative procedure for constructing a projection $P_*^\varepsilon(t)$ such that for every $n \in \mathbb{N}$ there is a constant $C_n < \infty$ improving (1.6) to

$$\left\| \left(\mathbf{1} - P_*^\varepsilon(t)\right) U^\varepsilon(t, t_0)\, P_*^\varepsilon(t_0) \right\| \leq C_n\, \varepsilon^n\, (1 + |t - t_0|)\,. \tag{1.23}$$

The projector $P_*^\varepsilon(t)$ satisfies

$$\|P_*(t) - P_*^\varepsilon(t)\| \leq C\,\varepsilon \tag{1.24}$$

for some constant $C < \varepsilon$ and allows for an asymptotic series expansion in ε,

$$P_*^\varepsilon(t) \asymp P_*(t) + \sum_{n=1}^{\infty} \varepsilon^n \, P_n(t) \,. \tag{1.25}$$

Remark 1.5. Note that we use Poincaré's definition of asymptotic power series throughout this monograph: the formal power series $\sum_{n=0}^{\infty} \varepsilon^n a_n$ is said to be the asymptotic power series for a function $f(\varepsilon)$ if for all $N \in \mathbb{N}$ there is a constant $C_N < \infty$ such that

$$|f(\varepsilon) - \sum_{n=0}^{N-1} \varepsilon^n a_n| \leq \varepsilon^N \, C_N \,,$$

where this relation is expressed symbolically through

$$f(\varepsilon) \asymp \sum_{n=0}^{\infty} \varepsilon^n a_n \,.$$

♢

Remark 1.6. Whenever $\frac{\mathrm{d}^n}{\mathrm{d}t^n} H(\tau) = 0$ for some $\tau \in \mathbb{R}$ and all $n \in \mathbb{N}$, then $P_*^\varepsilon(\tau) = P_*(\tau)$. ♢

Remark 1.7. Note that combining (1.23) and (1.24) yields

$$\big\| \big(\mathbf{1} - P_*(t)\big) \, U^\varepsilon(t, t_0) \, P_*(t_0) \, \big\| \leq C_n \, (\varepsilon + \varepsilon^n \, |t - t_0|)$$

for the non-tilted projectors $P_*(t)$. While the error $\mathcal{O}(\varepsilon)$ in (1.6) can not be improved without tilting the subspaces, the first order result for the non-tilted subspaces holds for much longer times. ♢

In concrete applications one can only compute a few leading terms in the expansion (1.25) of $P_*^\varepsilon(t)$. However, one is often not interested in explicitly determining $P_*^\varepsilon(t)$ for all $t \in \mathbb{R}$. Assume, e.g., that $H(t)$ varies only on some compact time interval $[t_1, t_2] \subset \mathbb{R}$, that the initial condition $\psi(t_0) \subset P_*(t_0)\mathcal{H}$ is specified at some time $t_0 < t_1$ and that one is interested in the solution of the Schrödinger equation $\psi(t_3) = U^\varepsilon(t_3, t_0)\psi(t_0)$ for times $t_3 > t_2$. Then according to (1.23) and Remark 1.6 one finds that

$$\|(\mathbf{1} - P_*(t_3))\psi(t_3)\| \leq C_n \, \varepsilon^n \, (1 + |t_3 - t_0|) \, \|\psi(t_0)\| \,.$$

This observation is due to [ASY$_1$], see also [ASY$_2$] and [KlSe], who consider the quantum Hall effect. Put differently, the part of the wave function that leaves the spectral subspace $P_*(t)\mathcal{H}$ of the Hamiltonian $H(t)$ during a compactly supported change in time is asymptotically smaller than any power of ε. For such a conclusion no explicit knowledge of $P_*^\varepsilon(t)$ is needed. However, one would like to obtain information on $\psi(t_3)$ beyond the mere fact that $\psi(t_3) \in P_*(t_3)\mathcal{H}$ up to small errors. To this end one approximates $U^\varepsilon(t, t_0)$ as in (1.21) through an effective time evolution

$$\mathcal{U}^{\varepsilon}(t)\, U^{\varepsilon}_{\mathrm{eff}}(t,t_0)\, \mathcal{U}^{\varepsilon *}(t_0)\,. \tag{1.26}$$

$\mathcal{U}^{\varepsilon}(t)$ now maps $P^{\varepsilon}_{*}(t)\mathcal{H}$ unitarily to the reference subspace $\mathbb{C}^{\ell}$ and thus the effective evolution (1.26) exactly transports the subspaces $P^{\varepsilon}_{*}(t)\mathcal{H}$.

The central object of adiabatic perturbation theory is the effective Hamiltonian $H^{\varepsilon}_{\mathrm{eff}}(t)$ generating $U^{\varepsilon}_{\mathrm{eff}}(t,t_0)$ as in (1.26). $H^{\varepsilon}_{\mathrm{eff}}(t)$ allows for an asymptotic expansion as

$$H^{\varepsilon}_{\mathrm{eff}}(t)_{\alpha\beta} \asymp E(t)\,\delta_{\alpha\beta} - \mathrm{i}\,\varepsilon\,\langle \varphi_{\alpha}(t), \dot{\varphi}_{\beta}(t)\rangle_{\mathcal{H}} + \sum_{n=2}^{\infty} \varepsilon^{n}\, H_n(t)_{\alpha\beta}\,,$$

starting with the first two orders as found in (1.20). In Chapter 4 we shall show that

$$H_2(t)_{\alpha\beta} = \frac{1}{2}\big\langle \dot{\varphi}_{\alpha}(t), \big(H(t)-E(t)\big)^{-1}\dot{\varphi}_{\beta}(t)\big\rangle_{\mathcal{H}}$$

and also explain how to calculate even higher orders.

As a net result we obtain the following. Consider the n^{th} order approximation to $H^{\varepsilon}_{\mathrm{eff}}(t)$,

$$H^{(n)}_{\mathrm{eff}}(t) = \sum_{j=0}^{n} \varepsilon^{n} H_n(t)\,,$$

and the corresponding effective evolution $U^{(n)}_{\mathrm{eff}}(t,t_0)$ on the reference space $\mathbb{C}^{\ell}$,

$$\mathrm{i}\,\varepsilon \frac{\mathrm{d}}{\mathrm{d}t}\, U^{(n)}_{\mathrm{eff}}(t,t_0) = H^{(n)}_{\mathrm{eff}}(t)\, U^{(n)}_{\mathrm{eff}}(t,t_0)\,, \quad U^{(n)}_{\mathrm{eff}}(t_0,t_0) = \mathbf{1}_{\mathbb{C}^{\ell}}\,. \tag{1.27}$$

Then there is a constant C_n such that

$$\big\| \big(U^{\varepsilon}(t,t_0) - \mathcal{U}^{\varepsilon *}(t)\, U^{(n)}_{\mathrm{eff}}(t,t_0)\, \mathcal{U}^{\varepsilon}(t_0)\big)\, P^{\varepsilon}_{*}(t_0)\big\| \leq C_n\, \varepsilon^{n}\, (1+|t-t_0|)\,. \tag{1.28}$$

If we are in the situation where $H(t)$ varies on the compact time interval $[t_1,t_2]$ only, then, according to (1.6), $P^{\varepsilon}_{*}(t) = P_{*}(t)$ and $\mathcal{U}^{\varepsilon}(t) = \mathcal{U}(t)$ are explicitly known for $t \notin [t_1,t_2]$. Hence it suffices to solve for the effective dynamics (1.27) on the reference subspace in order to obtain approximate solutions to the full Schrödinger equation up to any desired order in ε.

The scheme of computing asymptotic expansions for the projectors $P^{\varepsilon}_{*}(t)$, for the unitaries $\mathcal{U}^{\varepsilon}(t)$ and, in particular, for the effective Hamiltonian $H^{\varepsilon}_{\mathrm{eff}}(t)$ is called **time-adiabatic perturbation theory**.

Remark 1.8. We note that if $H(t)$ has an analytic continuation to some strip in the complex plane, then the error estimate in (1.23) can be improved to

$$\big\| \big(\mathbf{1} - P^{\varepsilon}_{*}(t)\big)\, U^{\varepsilon}(t,t_0)\, P^{\varepsilon}_{*}(t_0)\,\big\| \leq C\, \mathrm{e}^{-1/\varepsilon}\, (1+|t-t_0|)\,. \tag{1.29}$$

Rigorous accounts of this statement were first given in [JoPf$_2$, Nen$_1$]. In this monograph we will not be concerned with exponential estimates. This is because our focus is not on optimal asymptotic error estimates, but we will establish a general perturbative framework, which allows to calculate effective Hamiltonians up to any finite order. ♢

1.2 Space-adiabatic decoupling: examples from physics

Applications of the time-adiabatic theorem of quantum mechanics can be found in many different fields of physics. Indeed, the importance of a good understanding of adiabatic theory is founded in the fact that whenever a physical system contains degrees of freedom with well separated time-scales, or, equivalently, with well separated energy-scales, then adiabatic decoupling can be observed. A prominent application for the time-adiabatic theorem in mathematical physics is the quantum Hall effect [ASY$_1$, ASY$_2$].

In this section we discuss two examples from physics where the time-adiabatic theorem can be applied, but, as we shall argue, a space-adiabatic theorem provides a more natural and more detailed understanding of the physics. The first example is dynamics of molecules and usually comes under the name of time-dependent Born-Oppenheimer theory [BoOp, Ha$_1$, HaJo$_2$, SpTe, MaSo]. The second example is a single Dirac particle subject to weak external forces, modelling, e.g., an electron resp. positron in an accelerator, a cloud chamber or a similar device.

1.2.1 Molecular dynamics

Molecules consist of light electrons, mass m_e, and heavy nuclei, mass m_n which depends on the type of nucleus. Born and Oppenheimer [BoOp] wanted to explain some general features of molecular spectra and realized that, since the ratio $m_\mathrm{e}/m_\mathrm{n}$ is small, it could be used as an expansion parameter for the energy levels of the molecular Hamiltonian. This time-*independent* Born-Oppenheimer theory has been put on firm mathematical grounds by Combes, Duclos, and Seiler [Co, CDS], Hagedorn [Ha$_2$], and more recently by Klein, Martinez, Seiler and Wang [KMSW]. For a comparison of the methods and results we refer to Appendix C.

With the development of tailored state preparation and ultra precise time resolution there is a growing interest in understanding and controlling the dynamics of molecules, which requires an analysis of the solutions to the time-*dependent* Schrödinger equation, again exploiting that $m_\mathrm{e}/m_\mathrm{n}$ is small. For l nuclei with positions $x = \{x_1, \ldots, x_l\}$ and k electrons with positions $y = \{y_1, \ldots, y_k\}$ the molecular Hamiltonian is of the form

$$H_\mathrm{mol} = -\frac{\hbar^2}{2m_\mathrm{n}}\,\Delta_x - \frac{\hbar^2}{2m_\mathrm{e}}\,\Delta_y + V_\mathrm{e}(y) + V_\mathrm{en}(x,y) + V_\mathrm{n}(x) \tag{1.30}$$

with dense domain $H^2(\mathbb{R}^{3(l+k)}) \subset L^2(\mathbb{R}^{3(l+k)})$. For notational simplicity we ignore spin degrees of freedom and assume that all nuclei have the same mass m_n. The first and second term of H_mol are the kinetic energies of the nuclei and of the electrons, respectively. Electrons and nuclei interact via the static Coulomb potential. Therefore V_e is the electronic, V_n the nucleonic repulsion, and V_en the attraction between electrons and nuclei. V_e and V_n may also contain an external electrostatic potential.

Even for simple molecules as CO_2, which contains 3 nuclei and 22 electrons, a direct numerical treatment of the time-dependent Schrödinger equation

$$\mathrm{i}\,\hbar\,\frac{\mathrm{d}}{\mathrm{d}s}\,\psi(s) = H_{\mathrm{mol}}\,\psi(s)\,, \qquad \psi(s_0) = \psi_0 \in L^2(\mathbb{R}^{3(l+k)})\,, \tag{1.31}$$

is far beyond the capabilities of today's computers and will stay so for the foreseeable future. This is because of the high dimension of the configuration space, e.g. $3(l+k) = 75$ in the case of CO_2, and because of the fact that long microscopic times s must be considered in order to observe finite motion of the nuclei. As a consequence, good approximation schemes for solving (1.31) are of great interest for many fields of chemistry, chemical physics and biophysics. In the following we shall explain how the mechanism of adiabatic decoupling leads to such an approximation scheme in many relevant situations.

In atomic units ($m_{\mathrm{e}} = \hbar = 1$) the Hamiltonian (1.30) can be written more concisely as

$$H^{\varepsilon}_{\mathrm{mol}} = -\,\frac{\varepsilon^2}{2}\,\Delta_x + H_{\mathrm{e}}(x)\,, \tag{1.32}$$

where we introduced the small dimensionless parameter

$$\varepsilon = \sqrt{m_{\mathrm{e}}/m_{\mathrm{n}}}\,. \tag{1.33}$$

In (1.32) it is emphasized already that the nuclear kinetic energy will be treated as a "small perturbation". $H_{\mathrm{e}}(x)$ is the electronic Hamiltonian for given position x of the nuclei,

$$H_{\mathrm{e}}(x) = -\frac{1}{2}\,\Delta_y + V_{\mathrm{e}}(y) + V_{\mathrm{en}}(x,y) + V_{\mathrm{n}}(x)\,. \tag{1.34}$$

$H_{\mathrm{e}}(x)$ is a self-adjoint operator on the electronic Hilbert space $\mathcal{H}_{\mathrm{e}} = L^2(\mathbb{R}^{3k})$. Later on we shall assume some smoothness of $H_{\mathrm{e}}(x)$, which can be established easily if the electrons are treated as point-like and the nuclei have an extended, rigid charge distribution. Generically $H_{\mathrm{e}}(x)$ has, possibly degenerate, eigenvalues

$$E_1(x) < E_2(x) < E_3(x) < \dots\,,$$

which may terminate at the continuum edge $\Sigma(x)$. Thereby one obtains the band structure as plotted schematically in Figure 1.2. The discrete bands $E_j(x)$ may cross and possibly merge into the continuous spectrum as indicated in Figure 2.2.

If the kinetic energies of the nuclei and the electrons are of comparable magnitude, then one finds for the speeds

$$|v_{\mathrm{n}}| \approx (m_{\mathrm{e}}/m_{\mathrm{n}})^{1/2}|v_{\mathrm{e}}| = \varepsilon\,|v_{\mathrm{e}}|\,,$$

which means that the nuclei move much slower than the electrons.

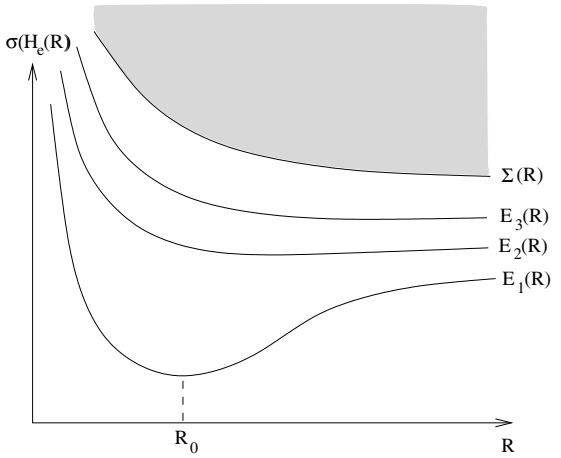

Fig. 1.2. The schematic spectrum of $H_{\mathrm{e}}(R)$ for a diatomic molecule as a function of the separation R of the two nuclei.

One might now argue that because of their large mass the nuclei are not only slow, but behave like classical particles with a configuration $q \in \mathbb{R}^{3l}$ moving slowly along some trajectory $q(t) = q(\varepsilon s)$. For the moment, we assume $q(t)$ to be given a priori. Then $H_{\mathrm{e}}(q(\varepsilon s))$ is a Hamiltonian with slow time variation and the time-adiabatic theory of Section 1.1 is applicable. If initially the electronic state is an eigenstate $\chi_j(q(0))$ of the electronic Hamiltonian $H_{\mathrm{e}}(q(0))$ corresponding to an isolated energy $E_j(q(0))$, i.e.

$$H_{\mathrm{e}}(q(0))\,\chi_j(q(0)) = E_j(q(0))\,\chi_j(q(0))\,,$$

then the time-adiabatic theorem states that at later times the solution $\psi(t)$ of

$$\mathrm{i}\,\varepsilon\,\frac{\mathrm{d}}{\mathrm{d}t}\,\psi(t) = H_{\mathrm{e}}(q(t))\,\psi(t)\,, \qquad \psi(0) = \chi_j(q(0)) \in L^2(\mathbb{R}^{3k}) \tag{1.35}$$

remains approximately an eigenstate of $H_{\mathrm{e}}(q(t))$ to the energy $E_j(q(t))$ also at later times, provided that $E_j(q(t))$ is separated by a gap from the remainder of the spectrum along the trajectory $q(t)$. The state of the electrons follows adiabatically the motion of the nuclei. Hence one argues that because of conservation of energy the influence of the electrons on the motion of the nuclei is well approximated through the effective potential energy $E_j(q)$ and that $q(t)$ is given as a solution to the classical equations of motion

$$\ddot{q}(t) = -\nabla E_j(q(t))\,. \tag{1.36}$$

The description of the dynamics of the nuclei inside molecules in terms of the simple classical equation of motion (1.36) is often called Born-Oppenheimer approximation in the chemical physics literature.

However, a priori the nuclei are quantum mechanical degrees of freedom and an approximation scheme as the one just described has to be derived starting from the full Schrödinger equation (1.31). But the Hamiltonian $H^{\varepsilon}_{\mathrm{mol}}$ of (1.32) is time-*independent* and we can only exploit that the nucleonic Laplacian carries a small prefactor. Since the nuclei are expected to move with a speed of order ε, their dynamics must be followed over microscopic times of order ε^{-1} to observe motion over finite distances. Hence, (1.31) becomes

$$\mathrm{i}\,\varepsilon\,\frac{\mathrm{d}}{\mathrm{d}t}\,\psi(t) = H^{\varepsilon}_{\mathrm{mol}}\,\psi(t)\,, \qquad \psi(t_0) = \psi_0 \in L^2(\mathbb{R}^{3(l+k)})\,, \tag{1.37}$$

where, as in (1.35), the factor ε in front of the time-derivative means that we switched to the slow time-scale.

The mathematical investigation of the time-dependent Born-Oppenheimer theory starting from (1.37) was initiated and carried out in great detail by Hagedorn. In his pioneering work [Ha$_1$] he constructs approximate solutions to (1.37), which are essentially of the form

$$\phi^{\varepsilon}_{q(t)} \otimes \chi_j(q(t))\,, \tag{1.38}$$

where $\phi^{\varepsilon}_{q(t)}$ is a suitable Gaussian wave packet sharply localized along a given classical trajectory $q(t)$ solving (1.36), and $\chi_j(x) \in \mathcal{H}_{\mathrm{e}}$ is an eigenfunction of $H_{\mathrm{e}}(x)$ for all $x \in \mathbb{R}^{3l}$.

More precisely, let $\psi^{\varepsilon}(t)$ be the true solution of (1.37) with the same initial condition as the approximate wave function (1.38), i.e. $\psi^{\varepsilon}(t_0) = \phi^{\varepsilon}_{q(t_0)} \otimes \chi_j(q(t_0))$. It follows from the results in [Ha$_1$] that, as long as the gap condition holds along $q(t)$, for each bounded time interval $I \ni t_0$ there is a constant $C_I < \infty$ such that for $t \in I$

$$\| \psi^{\varepsilon}(t) - \phi^{\varepsilon}_{q(t)} \otimes \chi_j(q(t)) \| \leq C_I \sqrt{\varepsilon}\,. \tag{1.39}$$

This result rigorously confirms the heuristic arguments involving the time-adiabatic theorem leading to (1.36), as it relates the "true" quantum mechanical description to the classical approximation. However, in Hagedorn's approach the "adiabatic and semiclassical limits are being taken simultaneously, and they are coupled [HaJo$_2$]".

Indeed, the proof of (1.39) relies on the time-adiabatic theorem, which, however, can only be applied because of the sharp localization of the nucleonic wave function. On the other hand there is no reason why adiabatic decoupling should only happen for well localized wave functions. After all, the underlying physical insight that the separation of time respectively energy scales leads to the adiabatic decoupling is completely unrelated to semiclassical behavior or localization of wave packets. Thus the concept of time-adiabatic decoupling as explained in Section 1.1 needs to be generalized to what was termed **space-adiabatic decoupling** in [SpTe].

Let us roughly explain the results of first order space-adiabatic theory for molecular dynamics as described by (1.37). Assume that $E_j(x)$ is isolated from the remainder of the spectrum of $H_{\rm e}(x)$ for some fixed j and, for simplicity, for all $x \in \mathbb{R}^{3l}$. Let $P_*(x)$ be the projection onto the eigenspace of $H_{\rm e}(x)$ corresponding to $E_j(x)$. Then

$$P_* = \int_{\mathbb{R}^{3l}}^{\oplus} \mathrm{d}x\, P_*(x)$$

defines a projection on the full Hilbert space

$$\mathcal{H} = L^2(\mathbb{R}^{3l}) \otimes L^2(\mathbb{R}^{3k}) = L^2(\mathbb{R}^{3l}, L^2(\mathbb{R}^{3k}))\,.$$

We term the subspace $P_*\mathcal{H}$ the band subspace corresponding to the energy band $E_j(\cdot)$. Note that $P_*\mathcal{H}$ is invariant for $H_{\rm e}$, i.e. $[P_*, H_{\rm e}] = 0$, although it is, in general, not a spectral subspace for $H_{\rm e}$.

However, $P_*\mathcal{H}$ is not invariant for the full molecular Hamiltonian, since

$$[H^\varepsilon_{\rm mol}, P_*] = [-\frac{\varepsilon^2}{2}\,\Delta_x, P_*] = -\frac{\varepsilon^2}{2}\big(\Delta P_* + 2\,\nabla P_* \cdot \nabla_x\big) \neq 0\,. \tag{1.40}$$

But, because of the spectral gap, one expects that the band subspace $P_*\mathcal{H}$ decouples from its orthogonal complement for small ε, i.e. for slow motion of the nuclei. Let

$$H^\varepsilon_{\rm diag} = P_*\, H^\varepsilon_{\rm mol}\, P_* + P_*^\perp\, H^\varepsilon_{\rm mol}\, P_*^\perp\,, \tag{1.41}$$

then $[H^\varepsilon_{\rm diag}, P_*] = 0$ and thus also

$$\Big[\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm diag}t/\varepsilon}, P_*\Big] = 0\,.$$

We shall show in Section 2.3 that for each $\lambda \in \mathbb{R}$ there is a constant $C < \infty$ such that

$$\Big\|\Big(\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm mol}t/\varepsilon} - \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm diag}t/\varepsilon}\Big)\; P(H^\varepsilon_{\rm mol} \leq \lambda)\Big\| \leq\; C\,\varepsilon\,(1+|t|)\,. \tag{1.42}$$

Here $P(H^\varepsilon_{\rm mol} \leq \lambda)$ denotes the spectral projection of $H^\varepsilon_{\rm mol}$ on energies smaller than λ. In particular, (1.42) shows that $P_*\mathcal{H}$ is an *approximately invariant subspace* of the full dynamics, i.e.

$$\Big\|\Big[\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm mol}t/\varepsilon},\, P_*\Big]\; P(H^\varepsilon_{\rm mol} \leq \lambda)\Big\| \leq\; C\,\varepsilon\,(1+|t|)\,. \tag{1.43}$$

Remark 1.9. The projection on finite total energies in (1.42) and in (1.43) is necessary, since otherwise the adiabatic decoupling could not be uniform. This is because no matter how small ε is, i.e. how heavy the nuclei are, without a bound on their kinetic energy they are not uniformly slow. ♢

Note the analogy between the space-adiabatic result (1.42) and the time-adiabatic result (1.10). The diagonal Hamiltonian $H^\varepsilon_{\mathrm{diag}}$ in (1.42) corresponds to the adiabatic Hamiltonian $H^\varepsilon_{\mathrm{a}}(t)$. Indeed, $H^\varepsilon_{\mathrm{a}}(t)$ as defined in (1.7) can be obtained, in complete analogy to (1.41), as

$$H^\varepsilon_{\mathrm{a}}(t) = P_*(t)\big(-\mathrm{i}\,\varepsilon\frac{\mathrm{d}}{\mathrm{d}t} + H(t)\big)P_*(t) + P_*^\perp(t)\big(-\mathrm{i}\,\varepsilon\frac{\mathrm{d}}{\mathrm{d}t} + H(t)\big)P_*^\perp(t)\,.$$

The kinetic energy of the nuclei in $H^\varepsilon_{\mathrm{mol}}$ plays the same role as the time-derivative played in the time-adiabatic setting. As we shall see in Chapter 2, also the structure of the proof of the space-adiabatic result (1.42) is analogous to the one of the time-adiabatic theorem.

Formally the only difference between the two settings, as presented up to now, is that in the time-adiabatic case one considers Hamiltonians fibered over the time-axis and in the space-adiabatic case one considers Hamiltonians fibered over the configuration space of the slow degrees of freedom. The terminology *space*-adiabatic partly originates in the latter observation.

Also in the space-adiabatic setting effective dynamics on the decoupled subspace $P_*\mathcal{H}$ are of primary interest. As in the time-adiabatic case one can map the subspace $P_*\mathcal{H}$ in a natural way to a reference space. Assume, for simplicity, that the eigenvalue $E_j(x)$ under consideration is simple, then the natural reference space is $L^2(\mathbb{R}^{3l})$. The unitary $\mathcal{U} : P_*\mathcal{H} \to L^2(\mathbb{R}^{3l})$ is given analogous to (1.17) as

$$\mathcal{U} = \int_{\mathbb{R}^{3l}}^{\oplus} \mathrm{d}x\, \mathcal{U}(x) = \int_{\mathbb{R}^{3l}}^{\oplus} \mathrm{d}x\, \langle \chi_j(x), \cdot\, \rangle\,, \tag{1.44}$$

where $\chi_j(x)$ is the eigenvector of $H_{\mathrm{e}}(x)$ to the eigenvalue $E_j(x)$. $\chi_j(x)$ is determined up to a x-dependent phase factor and for the moment we chose $\chi_j(x, y)$ real-valued, which fixes $\chi_j(x)$ up to a sign. This is possible, since $H_{\mathrm{e}}(x)$ is real.

The effective Hamiltonian for the nuclei now acts on the reference space $L^2(\mathbb{R}^{3l})$ and is obtained by unitarily mapping the on-band diagonal part of $H^\varepsilon_{\mathrm{mol}}$ to $L^2(\mathbb{R}^{3l})$,

$$H^\varepsilon_{\mathrm{eff}} = \mathcal{U}\, P_*\, H^\varepsilon_{\mathrm{mol}}\, P_*\, \mathcal{U}^* = -\frac{\varepsilon^2}{2}\,\Delta_x + E_j(x) + \mathcal{O}(\varepsilon^2)\,.$$

In analogy with (1.21) we shall find in Chapter 2 that

$$\Big\| \Big(\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{mol}}t/\varepsilon} - \mathcal{U}^*\, \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{eff}}t/\varepsilon}\, \mathcal{U} \Big)\; P_*\, P(H^\varepsilon_{\mathrm{mol}} \le \lambda) \Big\| \le\; C\,\varepsilon\,(1 + |t|) \tag{1.45}$$

for some constant $C < \infty$. Thus, in the presence of a spectral gap, the influence of the electrons on the dynamics of the nuclei is given through the effective potential energy $E_j(x)$. Put differently, (1.45) shows that if $\phi(t)$ is a solution of the Schrödinger equation

$$\mathrm{i}\,\varepsilon\,\frac{\mathrm{d}}{\mathrm{d}t}\,\phi(t) = H^{\varepsilon}_{\mathrm{eff}}\,\phi(t)\,, \qquad \phi(t_0) = \phi_0 \in \mathcal{H}_{\mathrm{n}}\,, \tag{1.46}$$

for the nuclei only, then an approximate solution of the full Schrödinger equation (1.37) can be obtained by multiplying $\phi(t)$ with the corresponding electronic eigenstate $\chi_j(x)$, i.e. through

$$\psi(t,x,y) = (\mathcal{U}^*\phi)(t,x,y) = \phi(t,x)\,\chi_j(x,y)\,.$$

Note that $\psi(t) \in \mathcal{H}$ constructed this way is *not* a product wave function as (1.38) is.

Remark 1.10. It is straight forward to obtain approximate solutions of the effective Schrödinger equation (1.46) by means of standard semiclassical techniques, since $H^{\varepsilon}_{\mathrm{eff}}$ is a standard semiclassical operator, cf. Chapter 2 and Chapter 3. In particular, one can recover the results of Hagedorn [Ha$_1$] by constructing semiclassical wave packets for (1.46). ♢

In summary we found that first-order space-adiabatic theory for molecular Hamiltonians can be formulated in close analogy to the first-order time-adiabatic theory of Section 1.1. However, it turns out that this is not possible anymore for higher order space-adiabatic decoupling and new concepts and tools are needed. Indeed, once the general framework of Chapter 3 is developed, it becomes clear why time-adiabatic theory is special and, in particular, simple, when it comes to higher orders. As the next example from physics will show, even first-order space-adiabatic theory requires new concepts, in general.

1.2.2 The Dirac equation with slowly varying potentials

While there is still no complete agreement on the physical significance of the one particle Dirac equation, it can certainly be used to describe the motion of electrons or positrons in sufficiently weak external electromagnetic fields in good approximation. We have in mind situations as in storage rings, accelerators, mass spectrometers or cloud chambers. This is the physical regime which we consider in the following and as standard reference for the mathematics and the physics of the Dirac equation we refer to the book by Thaller [Th].

The free Dirac Hamiltonian

$$H_{\mathrm{D0}} = -\mathrm{i}\,\boldsymbol{\alpha}\cdot\nabla_y + \boldsymbol{\beta}\,m \tag{1.47}$$

with domain $H^1(\mathbb{R}^3,\mathbb{C}^4) \subset \mathcal{H} := L^2(\mathbb{R}^3,\mathbb{C}^4)$ is self-adjoint. We use units where $\hbar = c = 1$ and m is the mass of an electron. For the Dirac matrices $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$ we chose the standard representation

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}\,, \qquad \boldsymbol{\beta} = \begin{pmatrix} \mathbf{1}_{\mathbb{C}^2} & 0 \\ 0 & -\mathbf{1}_{\mathbb{C}^2} \end{pmatrix}\,,$$

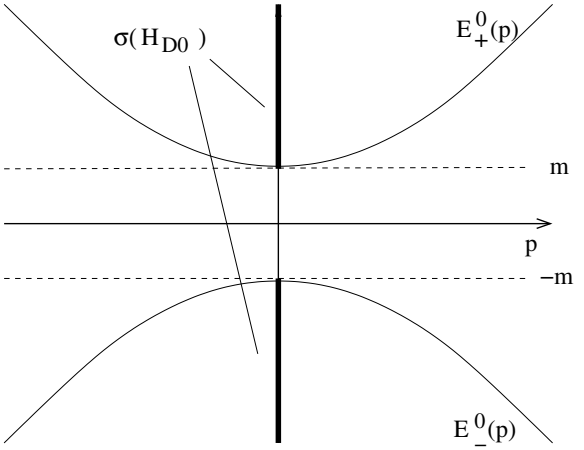

Fig. 1.3. The spectrum of the free Dirac Hamiltonian H_{D0} as projection of the fibered spectrum of $H_{\mathrm{D0}}(p)$ on the energy axis.

where $\boldsymbol{\sigma} = (\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3)$ denotes the vector of the Pauli spin matrices,

$$\boldsymbol{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.48}$$

The free Dirac Hamiltonian is most conveniently studied in Fourier representation and with $\mathcal{F} : L^2(\mathbb{R}^3_y) \to L^2(\mathbb{R}^3_p)$ denoting Fourier transformation one finds

$$H_{\mathrm{D0}}(p) := \mathcal{F}\, H_{\mathrm{D0}}\, \mathcal{F}^{-1} = \boldsymbol{\alpha} \cdot p + \boldsymbol{\beta}\, m\,.$$

Hence $H_{\mathrm{D0}}(p)$ acts as multiplication with a hermitian matrix valued function. The eigenvalues of the four by four matrix $H_{\mathrm{D0}}(p)$ are easily found to be

$$E^0_{\pm}(p) = \pm\sqrt{p^2 + m^2}\,,$$

both two-fold degenerate. The corresponding eigenprojections are

$$P^0_{\pm}(p) = \frac{1}{2}\left(\mathbf{1} + \frac{H_{\mathrm{D0}}(p)}{E^0_{\pm}(p)}\right).$$

The energy bands $E^0_+(p)$ and $E^0_-(p)$ are not only separated by a gap pointwise in p, but their projections on the energy axis are, as indicated in Figure 1.3, disjoint,

$$\inf_{p\in\mathbb{R}^3} E^0_+(p) = m > -m = \sup_{p\in\mathbb{R}^3} E^0_-(p)\,. \tag{1.49}$$

Thus, in contrast to the situation of the electronic Hamiltonian $H_{\mathrm{e}}(x)$ of the previous section, the band subspaces $P^0_{\pm}$ are spectral subspaces of H_{D0}.

States in $P^0_+\mathcal{H}$ are called electronic states or just electrons and states in $P^0_-\mathcal{H}$ are called positronic states or just positrons. For the free Dirac dynamics this notion makes perfectly sense, since $P^0_+\mathcal{H}$ and $P^0_-\mathcal{H}$ are invariant under the dynamics generated by $H_{\mathrm{D}0}$. Electrons stay electrons and positrons stay positrons.

In order to describe the dynamics of electrons and positrons in a weak and slowly varying external electric field $E = -\nabla\phi$ one adds to (1.47) the potential $\phi : \mathbb{R}^3 \to \mathbb{R}$,

$$H^\varepsilon_{\mathrm{D}\phi} = -\mathrm{i}\,\boldsymbol{\alpha}\cdot\nabla_y + \boldsymbol{\beta}\,m + \phi(\varepsilon\, y)\,, \tag{1.50}$$

where $\varepsilon > 0$ now controls the scale of variation of the potential ϕ. To keep formulas short we absorbed the charge of the electron into the potential. Switching again to Fourier representation, we obtain

$$H^\varepsilon_{\mathrm{D}\phi} = H_{\mathrm{D}0}(p) + \phi(\mathrm{i}\,\varepsilon\nabla_p) \tag{1.51}$$

and recover a structure quite similar to the one found in (1.32) for the molecular Hamiltonian, but with the roles of position and momentum interchanged.

One could now proceed as in the Born-Oppenheimer example. We would find that the spectral subspaces $P^0_\pm\mathcal{H}$ of $H_{\mathrm{D}0}$ are still approximately invariant under the dynamics generated by $H^\varepsilon_{\mathrm{D}\phi}$, although $P^0_\pm\mathcal{H}$ are no longer spectral subspaces of $H^\varepsilon_{\mathrm{D}\phi}$ once the gap in the spectrum of $H^\varepsilon_{\mathrm{D}\phi}$ closes. More precisely, the result of such an analysis would be that

$$\left[\,\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{D}\phi}t/\varepsilon},\, P^0_\pm\,\right] = \mathcal{O}(\varepsilon(1+|t|))\,,$$

and that on the electronic resp. positronic subspaces the dynamics are generated by effective Hamiltonians given through

$$H^\varepsilon_{\mathrm{eff}\,\pm} = \pm\sqrt{p^2+m^2} + \phi(\mathrm{i}\,\varepsilon\nabla_p)\,.$$

However, eventually one would like to consider also slowly varying external magnetic fields and then (1.51) becomes

$$H^\varepsilon_{\mathrm{D}} = H_{\mathrm{D}0}\big(p - A(\mathrm{i}\,\varepsilon\nabla_p)\big) + \phi(\mathrm{i}\,\varepsilon\nabla_p)\,, \tag{1.52}$$

where $A : \mathbb{R}^3 \to \mathbb{R}^3$ is the vector potential of an external magnetic field $B = \nabla\times A$. The Hamiltonian (1.52) does *not* have the same structure

$$H^\varepsilon = \int_{\mathbb{R}^n}^{\oplus} \mathrm{d}\xi\, H_0(\xi) + f(\mathrm{i}\,\varepsilon\nabla_\xi)\otimes\mathbf{1}$$

as H_{mol} or $H_{\mathrm{D}\phi}$ anymore. I.e., it is not the sum of an operator which is fibered over some configuration space plus a perturbation which acts on the slow degrees of freedom only.

The natural way to think of (1.52) is that of being "fibered" over phase space in the sense that

$$H_{\mathrm{D}}(q,p) = \boldsymbol{\alpha}\cdot\big(p - A(q)\big) + \boldsymbol{\beta}m + \phi(q) \tag{1.53}$$

is an operator valued function on phase space, $H_{\mathrm{D}}(\cdot) : \mathbb{R}^6 \to \mathcal{L}(\mathbb{C}^4)$, i.e. it depends on position q and momentum p of the particle. The full Hamiltonian $H_{\mathrm{D}}^{\varepsilon}$ acting on $L^2(\mathbb{R}^3,\mathbb{C}^4)$ is obtained by replacing in $H_{\mathrm{D}}(q,p)$ each occurrence of q with the operator $\mathrm{i}\,\varepsilon\nabla_p$ and each p with the operator of multiplication by p. The operator $\widehat{H}_{\mathrm{D}} = H_{\mathrm{D}}^{\varepsilon}$ obtained this way is called the **quantization** of the **symbol** H_{D}, a relation graphically expressed through the $\widehat{\ }$. Note, in particular, that all operators with a $\widehat{\ }$ depend on ε by construction. For the special case of $H_{\mathrm{D}}(q,p)$ no ambiguities from operator ordering arise. In general, however, one has to specify a rule and we shall adopt the Weyl-ordering throughout, cf. Appendix A.

The eigenvalues of the symbol $H_{\mathrm{D}}(q,p)$ are now functions on phase space $\mathbb{R}^6$ and explicitly given as

$$E_{\pm}(q,p) = E_{\pm}^0\big(p - A(q)\big) + \phi(q) = \pm\sqrt{(p-A(q))^2 + m^2} + \phi(q)\,.$$

While, in general, the situation will not be as in (1.49) anymore, i.e. the full Hamiltonian $\widehat{H}_{\mathrm{D}}$ will not have a spectral gap, still the eigenvalues of the symbol $H_{\mathrm{D}}(q,p)$ are separated uniformly over phase space by a gap,

$$\inf_{(q,p)\in\mathbb{R}^6}\big(\,E_+(q,p) - E_-(q,p)\,\big) = 2m > 0\,.$$

Naively one might hope that the subspaces $P_{\pm}^0\mathcal{H}$ which we identified with electrons and positrons are approximately invariant also under the dynamics generated by $\widehat{H}_{\mathrm{D}}$. But not only that the space-adiabatic theory as developed up to now is not applicable anymore, it turns out that this naive hope is actually wrong.

However, a slightly more educated guess gives the correct result. Let $P_{\pm}(q,p)$ be the spectral projections of $H_{\mathrm{D}}(q,p)$ corresponding to $E_{\pm}(q,p)$ and $\widehat{P}_{\pm}$ their Weyl-quantizations. And indeed, we shall show in Chapter 4 that for arbitrary $n\in\mathbb{N}$

$$\Big[\,\mathrm{e}^{-\mathrm{i}\widehat{H}_{\mathrm{D}}s},\,\widehat{P}_{\pm}\,\Big] = \mathcal{O}(\varepsilon + \varepsilon^n|s|)\,. \tag{1.54}$$

However, while $\widehat{P}_+$ and $\widehat{P}_-$ are self-adjoint operators on $\mathcal{H}$ they are only approximately projectors,

$$\|\,\widehat{P}_{\pm}^2 - \widehat{P}_{\pm}\,\| = \mathcal{O}(\varepsilon)\,,$$

and thus do not define subspaces. One can now use a trick due to Nenciu, cf. Chapter 3, and construct orthogonal projectors $Q_{\pm}^{\varepsilon}$ such that

$$\| Q^\varepsilon_\pm - \widehat{P}_\pm \| = \mathcal{O}(\varepsilon)\,.$$

Together with (1.54) we obtain

$$\left[\mathrm{e}^{-\mathrm{i}\widehat{H}_\mathrm{D} s},\, Q^\varepsilon_\pm \right] = \mathcal{O}(\varepsilon + \varepsilon^n |s|)\,, \tag{1.55}$$

i.e. $Q^\varepsilon_\pm \mathcal{H}$ are approximately invariant subspaces associated with the eigenvalue bands $E_\pm(q,p)$ of the symbol of $\widehat{H}_\mathrm{D}$.

Remark 1.11. Since the subspaces $Q^\varepsilon_\pm \mathcal{H}$ are still associated with the energy bands $E_\pm(q,p)$, it seems natural to call – in the presence of weak fields – states in $Q^\varepsilon_+ \mathcal{H}$ electrons and states in $Q^\varepsilon_- \mathcal{H}$ positrons. In fact we shall see in Section 4.1 that states in $Q^\varepsilon_+ \mathcal{H}$ have an effective dynamics as expected for electrons and states in $Q^\varepsilon_- \mathcal{H}$ as expected for positrons. ♢

Based on the powerful machinery of parameter-dependent pseudodifferential calculus it is not only possible to generalize the first-order space-adiabatic theory to situations like the Dirac equation with external magnetic fields, but it will also be at the basis for a general higher-order space-adiabatic theory. While this is the topic of Chapter 3, let us end this section with a short example for the physical relevance of effective Hamiltonians.

The so called T-BMT equation was derived by Thomas [Tho] and, in a more general form, by Bargmann, Michel and Telegdi [BMT] on purely classical grounds as the simplest Lorentz invariant equation for the spin dynamics of a classical relativistic particle. It is of great physical importance, since it was used to compute the anomalous magnetic moment of the electron from experimental data before the invention of particle traps. As a consequence the experimental verification of the outstanding prediction of QED, the anomalous g-factor, relied on the T-BMT equation.

We shall present a rigorous derivation of the T-BMT equation as the adiabatic and the semiclassical limit of the Dirac equation in Section 4.1.3. However, in order to give a motivation for our interest in effective Hamiltonians already at this place, let us apply once again the time-adiabatic theorem, this time to the Dirac equation. As in the case of molecular dynamics assume that a classical trajectory $(q(t), p(t))$ of say a relativistic electron is given. I.e., $(q(t), p(t))$ is a solution to the classical equations of motion

$$\dot{q}(t) = \nabla_p E_+\big(q(t), p(t)\big)\,, \quad \dot{p}(t) = -\nabla_q E_+\big(q(t), p(t)\big)\,,$$

with initial conditions $(q(0), p(0)) = (q_0, p_0) \in \mathbb{R}^6$. If we insert such a solution into the Dirac Hamiltonian (1.53), we obtain the time-dependent Hamiltonian

$$H_\mathrm{D}(t) = \boldsymbol{\alpha} \cdot \big(\, p(t) - A(q(t))\big) + \boldsymbol{\beta} m + \phi(q(t))$$

acting on spin-space $\mathbb{C}^4$. Being an electron, its spin state is initially given through some $\psi_0 \in P_+(q_0, p_0)\mathbb{C}^4$, and, heuristically, its time-evolution should be given as the solution of

$$\mathrm{i}\,\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\,\psi(t) = H_{\mathrm{D}}(t)\,\psi(t)\,, \qquad \psi(0) = \psi_0\,. \tag{1.56}$$

The time-adiabatic theorem asserts that for small ε, i.e. for slowly varying external potentials, the spin-state $\psi(t)$ remains in the subspace $P_+(q(t),p(t))\mathbb{C}^4$, i.e. the electron remains an electron and almost no positronic components are created. However, the subspace $P_+(q(t),p(t))\mathbb{C}^4$ is two-dimensional and $P_+(q(t),p(t))\,\psi(t)$ is nothing but the spin of the electron, which, according to Theorem 1.4 can be approximated through a simple effective dynamics.

The reference space for the effective dynamics is $\mathbb{C}^2$ and the effective dynamics depends on the way we identify $P_+(q(t),p(t))\mathbb{C}^4$ with $\mathbb{C}^2$, i.e. on the choice of an orthonormal basis in $P_+(q(t),p(t))\mathbb{C}^4$. Such a choice has to be motivated on physical grounds and a natural choice are the eigenvectors of the z-component of the "mean-spin" operator $\mathbf{S}(q,p)$, which commutes with $H_{\mathrm{D}}(q,p)$, cf. [FoWo, Sp$_1$]. Let $e(v) = \sqrt{v^2+m^2}$, $v \in \mathbb{R}^3$, and

$$\psi_{+z}(v) = \frac{1}{N(v)}\begin{pmatrix} e(v)+m \\ 0 \\ v_z \\ v_x + \mathrm{i}v_y \end{pmatrix}\,, \quad \psi_{-z}(v) = \frac{1}{N(v)}\begin{pmatrix} 0 \\ e(v)+m \\ v_x - \mathrm{i}v_y \\ -v_z \end{pmatrix}\,,$$

where the normalization is given through $N(v) = \sqrt{2e(v)(e(v)+m)}$. Then

$$H_{\mathrm{D}}(q,p)\,\psi_{\pm z}\big(p-A(q)\big) = E_+(q,p)\,\psi_{\pm z}\big(p-A(q)\big)$$

and

$$\mathbf{S}_z(q,p)\,\psi_{\pm z}\big(p-A(q)\big) = \pm\tfrac{1}{2}\,\psi_{\pm z}\big(p-A(q)\big)\,.$$

Thus we define as in (1.17)

$$\mathcal{U}(t) = \Big|\begin{pmatrix}1\\0\end{pmatrix}\Big\rangle\Big\langle\psi_{+z}\big(p(t)-A(q(t))\big)\Big| \;+\; \Big|\begin{pmatrix}0\\1\end{pmatrix}\Big\rangle\Big\langle\psi_{-z}\big(p(t)-A(q(t))\big)\Big|\,,$$

and obtain as effective Hamiltonian, after a lengthy but straightforward computation,

$$H_+(t) = E_+\big(q(t),p(t)\big)\,\mathbf{1}_{\mathbb{C}^2} + \varepsilon\,\Omega\big(q(t),p(t)\big)\cdot\boldsymbol{\sigma}$$

with

$$\Omega(q,p) = \frac{1}{e(v)}\left(B(q) - \frac{v\times E(q)}{e(v)+m}\right)\,, \qquad v = p - A(q)\,.$$

In summary we conclude that we can approximately calculate the spin dynamics of an electron along a given classical relativistic trajectory by solving

$$\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\,\chi(t) = \Omega\big(q(t),p(t)\big)\cdot\boldsymbol{\sigma}\,\chi(t)\,, \qquad \chi(0) = \chi_0 \in \mathbb{C}^2\,. \tag{1.57}$$

This is because according to Theorem 1.4

$$\psi(t) := \mathrm{e}^{-iE_+(q(t),p(t))t/\varepsilon}\,\mathcal{U}^*(t)\,\chi(t)$$

is then an approximate solution to (1.56) with $\psi_0 = \mathcal{U}^*(0)\chi_0$. However, (1.57) is nothing but the T-BMT equation for the spin of a classical relativistic electron. This derivation of the T-BMT equation (1.57) showed that the effective Hamiltonian carries important physical information also beyond the leading order term given through the so called Peierl's substitution. A severe drawback of the derivation of the T-BMT equation via the time-adiabatic theorem is that, even at higher orders, it is impossible to see a back-reaction of the spin-dynamics on the translational motion. This is because we must a priori prescribe the classical trajectory of the particle along which we choose to compute the evolution of its spin. Such a simple minded adiabatic approximation thus will never explain why an electron beam is split in a Stern-Gerlach magnet because of spin. This problem, as we will see in Section 4.1.2, is solved once we switch to the *space*-adiabatic setting.

Thus one of our main interests in this monograph will be a general space-adiabatic perturbation theory which allows us to systematically compute effective Hamiltonians.

1.3 Outline of contents and some left out topics

We conclude the introduction with a brief outline of the contents of every chapter and with some remarks on related topics which had to be left out.

Chapter 2: First order adiabatic theory

Section 2.1 contains the proof of the first order time-adiabatic theorem as going back basically to Kato [Ka_2] and Nenciu [Nen_4]. The case of regular eigenvalue crossings is included as a corollary. The presentation is such that the generalization to the first order space-adiabatic theorem is straightforward. In Section 2.2 the first order space-adiabatic theorem is formulated for a certain class of adiabatic problems, namely for perturbations of fibered Hamiltonians. This is done under simplifying assumptions in order to provide a pedagogical introduction. The idea to translate the time-adiabatic theorem to a space-adiabatic version was first used by Hövermann, Spohn and Teufel [HST] in the context of the semiclassical limit in periodic structures and subsequently modified and applied to the semiclassical limit of dressed electrons by Teufel and Spohn [TeSp] and to the derivation of the time-dependent Born-Oppenheimer approximation in molecular dynamics by Spohn and Teufel [SpTe]. Since the Born-Oppenheimer approximation is not only of relevance to many fields, but is at the same time conceptually very simple, the results from [SpTe] are presented and elaborated on in Section 2.3. As a new application we discuss the problem of quantum motion constrained to a submanifold of configuration space in Section 2.4 and compare the results to those known for the analogous classical problem.

In principle the method of Chapter 2 becomes obsolete through the introduction of the more general scheme as to be developed in Chapter 3. However, the method of Chapter 2 is elementary and also more flexible when it comes to regularity of the symbol of H or to localization in phase space. Last but not least it is this elementary method which is picked up again in Chapter 6 where adiabatic decoupling without gap-condition is considered.

Chapter 3: Space-adiabatic perturbation theory

This chapter contains the general scheme of space-adiabatic perturbation theory dealing with the abstract problem formulated in (1.1). The theory uses in its formulation and its proofs pseudodifferential operators with operator-valued symbols and a short presentation of the relevant material can be found in Appendix A. Chapter 3 is based on Panati, Spohn, Teufel [PST$_1$].

In our scheme the construction of the effective dynamics for the slow degrees of freedom follows three steps. First the approximately invariant subspaces corresponding to isolated spectral bands of the symbol H are constructed in Section 3.1. As to be explained there, this construction has some history. Here we only mention that we will use an approach to the construction of the approximately invariant subspace which is due to Nenciu and Sordoni [NeSo].

As a second step the approximately invariant subspace, which is a rather complicated and ε-dependent object, is mapped to a reference subspace which is simple and adapted to the problem. The unitary operator which intertwines the almost invariant subspace with the simple reference subspace is constructed in Section 3.2.

The effective Hamiltonian for the slow degrees of freedom is defined as the restriction of the full Hamiltonian to the almost invariant subspace mapped to the reference subspace. This procedure allows to compute the effective Hamiltonian as acting on the reference subspace to arbitrary order in ε. As to be shown in Section 3.3 and Section 3.4, the leading orders of this expansion provide very relevant information about the dynamics of the slow degrees of freedom.

In many cases the effective Hamiltonian is the quantization of a matrix-valued symbol with scalar principal symbol. Therefore we review in Section 3.4 some results on semiclassics for matrix-valued Hamiltonians. Moreover the geometrical interpretation of the subprincipal symbol of the effective Hamiltonian as coming partly from the famous Berry connection is most conveniently discussed in the context of the semiclassical limit.

Chapter 4: Applications and extensions

Space-adiabatic perturbation theory as developed in Chapter 3 can be directly applied to the Dirac equation with slowly varying external potentials.

From the explicit expansion of the effective Hamiltonian to first order we derive, in particular, the T-BMT equation. In addition we also derive the first order corrections to the semiclassical equations of motion of a Dirac particle including back-reaction of spin onto the translational dynamics.

As already mentioned in Section 1.2, adiabatic decoupling for the molecular Hamiltonian can only hold after imposing suitable energy cutoffs. In Section 4.2 we briefly discuss how to modify the general theory such that also the Born-Oppenheimer approximation is covered and calculate the effective Hamiltonian including second order corrections. Our results generalize the expression for the effective Hamiltonian for the Born-Oppenheimer approximation found by Littlejohn and Weigert [LiWe$_1$]. We also remark that the time-dependent Born-Oppenheimer approximation with exponentially small error estimates was discussed by Martinez and Sordoni in [MaSo].

In Section 4.3 we reconsider the time-adiabatic theorem based on the general framework. Also here we are able to compute the effective Hamiltonian including second order corrections.

We close Chapter 4 with two heuristic sections relevant to applications of the theory. In Section 4.4 we discuss the question "How good is the adiabatic approximation in a concrete problem ?" and in Section 4.5 we study the effective Born-Oppenheimer Hamiltonian near a conical eigenvalue crossing.

Chapter 5: Dynamics in periodic structures

As a not so obvious application of space-adiabatic perturbation theory we discuss the dynamics of an electron in a periodic potential based on Panati, Spohn, Teufel [PST$_3$]. Indeed it requires considerable insight into the problem and some analysis to even formulate this question as a space-adiabatic problem. More precisely the general form (1.1) is achieved only after a suitable Bloch-Floquet transformation, which is discussed in Section 5.1. In Section 5.2 the general scheme of Chapter 3 is applied, however, with several technical innovations. While formally the problem has the general form (1.1), a rigorous treatment can be based only on a Weyl calculus for a certain class of equivariant symbols acting on equivariant functions. Such a calculus is developed in Appendix B. Furthermore the problem of the Bloch electron also exemplifies the treatment of unbounded-operator-valued symbols within adiabatic perturbation theory. In Section 5.3 we derive the first order corrections to the semiclassical model of solid states physics. We do not only rigorously reproduce the correction terms recently found in [ChNi$_1$, ChNi$_2$, SuNi], but also find an additional term which has been missed so far.

Chapter 6: Adiabatic decoupling without spectral gap

Adiabatic decoupling without spectral gap has been considered only quite recently. Time-adiabatic theorems without gap condition were proven independently by Bornemann [Bor] and by Avron and Elgart [AvEl$_1$]. Section 6.1

contains a version of the result from [AvEl$_1$] with improved error estimates, where, at the same time, the proof is simplified considerably. This result appeared in [Te$_2$].

In Section 6.2 the techniques from [Te$_2$] are translated to perturbations of fibered Hamiltonians and a general space-adiabatic theorem without gap condition is established. As an application of this result effective N-body dynamics for the massless Nelson model are derived in Section 6.3. The latter result appeared in [Te$_1$].

Appendices

Appendix A reviews some results from the theory of parameter dependent pseudodifferential operators with operator-valued symbols. Chapter 3 heavily relies on the notation and the calculus introduced here.

In order to translate the scheme developed in Chapter 3 to the Schrödinger equation with a short scale periodic potential, a Weyl calculus for certain τ-equivariant symbols must be developed. This is the content of Appendix B.

Of course we compare our method to related ones throughout this monograph whenever appropriate. Still, for the convenience of the interested reader, we devote Appendix C to a discussion of related approaches. More precisely in the context of time-independent Born-Oppenheimer theory a powerful method for deriving effective Hamiltonians was developed in [CDS, KMSW] and also applied to the Bloch electron in [GMS]. For an abstract account of the method see Martinez [Ma$_2$]. As to be explained in Appendix C this scheme gives results which are somewhat disjoint from ours.

Mainly in the context of Born-Oppenheimer approximation Hagedorn [Ha$_1$, Ha$_3$, Ha$_4$] and Hagedorn and Joye [HaJo$_1$, HaJo$_2$] obtained very strong results on the propagation of coherent states, which we shortly comment in Appendix C. Since matrix-valued Wigner measures [GMMP] become more and more popular in the context of the partial semiclassical limit problem (1.1), we also comment on this approach.

Topics left out

We conclude this summary with a list of closely related topics, which had to be left out completely in this monograph.

Up to Chapter 6 we always assume a gap condition, at least locally in the configuration space of the slow degrees of freedom. In the presence of eigenvalue crossings our results permit to derive an effective Hamiltonian for a group of bands, inside of which the crossing occurs. However, the study of such an effective Hamiltonian is in itself a veritable task. Much work has been spent in order to study model Hamiltonians displaying different types of eigenvalue crossings, among which we mention only some recent work [Ha$_3$, HaJo$_1$, CLP, FeGe, FeLa, Col$_1$, Col$_2$, LaTe]. While we shall touch this circle of

problems only shortly in Section 4.5, we emphasize again that our results give a rigorous justification for the reduction of a full Hamiltonian, like the one in molecular dynamics, to the model Hamiltonians as studied in the literature on crossings. A short discussion of this point can be found in [FeLa].

Physically one expects that transitions between adiabatically decoupled subspaces are exponentially small in the parameter ε, cf. Remark 1.8. Exponential error estimates were established first in the time-adiabatic setting in [JoPf$_2$, Nen$_1$]. For certain model systems it is even possible to study the exponentially small transition amplitudes explicitly, cf. [LiBe, BeLi$_1$, Be$_2$]. In the space-adiabatic setting exponential error estimates were obtained in [HaJo$_2$, MaSo, NeSo] for Born-Oppenheimer type Hamiltonians. We refrain from proving such exponential error estimates, since our focus is on adiabatic *perturbation* theory, i.e. we are interested in explicit expansions of effective Hamiltonians to some finite order, which, as we shall see, carry important physical information.

Still the applications based on our results on effective Hamiltonians are multifaceted and we will discuss only a few. An important omission is the computation of so called g-factors. This is not only of central relevance for spinning particles coupled to the quantized radiation field, cf. [PST$_2$], but also in solid state physics, where the details will be given in [PST$_3$]. Also in scattering theory asymptotic expansions of the S-matrix can be based on effective Hamiltonians, cf. [NeSo].

Another interesting aspect of adiabatic theory are efficient algorithms for a numerical treatment of adiabatic problems. Naturally the goal of such numerical computations is to capture correctly the small but finite transitions between the adiabatically decoupled subspaces. For a careful numerical analysis and efficient algorithms for the standard time-adiabatic problem including avoided crossings we refer to [JaLu]. A semiclassical model for a Born-Oppenheimer type Hamiltonian with a conical crossing is derived and tested numerically in [LaTe].

2 First order adiabatic theory

The present chapter deals with the leading order adiabatic theory, i.e. error terms are of first order in the parameter ε. As a first step we recall in Section 2.1 the proof of the classical time-adiabatic theorem as described in the introduction and its generalization to regular crossings of eigenvalues. The presentation is such that the generalization to a certain class of space-adiabatic problems, namely perturbations of fibered Hamiltonians, becomes straightforward. This is explained in Section 2.2 under rather simplifying assumptions. We refrain from proving the result for perturbations of fibered Hamiltonians in greater generality for two reasons. On the one hand the general theory to be developed in Chapter 3 will in principle cover also this special class of problems, but requires more stringent assumptions on the Hamiltonian. Thus the theory to be developed in this chapter can be seen as a last resort when the general scheme can not be applied directly. This is the case for the Born-Oppenheimer approximation as explained in the introduction and hence we elaborate on this example in Section 2.3 in order to demonstrate the flexibility of the present approach. On the other hand we will return to the setting of perturbations of fibered Hamiltonians once we remove the gap condition in Chapter 6. There we will establish a general result, the proof of which can easily be translated back to the case with gap.

We remark that the idea to be developed in this chapter was applied in a variety of different physical contexts: motion of electrons in periodic potentials with a weak external electric field [HST], the dynamics of dressed electrons under the influence of a slowly varying external potential [TeSp] and the Born-Oppenheimer approximation [SpTe].

2.1 The classical time-adiabatic result

In this section we state and prove a slightly more general version of the time-adiabatic theorem compared to Theorem 1.2 of the introduction. In particular, we allow for unbounded Hamiltonians $H(t)$ and start with a proposition concerning the nontrivial question of the existence of a unitary propagator in this case.

S. Teufel: LNM 1821, pp. 33–69, 2003.

Proposition 2.1. *For some open interval $J \subseteq \mathbb{R}$ let $H(t)$, $t \in J$, be a family of self-adjoint operators on some Hilbert space $\mathcal{H}$ with a common dense domain $\mathcal{D} \subset \mathcal{H}$, equipped with the graph norm of $H(t)$ for some $t \in J$, such that*

(i) $H(\cdot) \in C^1_{\mathrm{b}}(J, \mathcal{L}(\mathcal{D}, \mathcal{H}))$,
(ii) $H(t) \geq C$ *for all* $t \in J$ *and some* $C > -\infty$.

Then there exists a unitary propagator U^ε, cf. Definition 1.1, such that for $t, t_0 \in J$ and $\psi_0 \in \mathcal{D}$ a solution to the time-dependent Schrödinger equation

$$\mathrm{i}\,\varepsilon \frac{\mathrm{d}}{\mathrm{d}t}\,\psi(t) = H(t)\,\psi(t)\,, \quad \psi(t_0) = \psi_0\,.$$

is given through $\psi(t) = U^\varepsilon(t, t_0)\psi_0$.

Proposition 2.1 is an immediate consequence of the general result on contraction semigroups, cf. Theorem X.70 in [ReSi$_2$].

The first proof of the time-adiabatic theorem is due to Born and Fock [BoFo] and important advances were achieved by Kato [Ka$_2$], Garrido [Ga] and Nenciu [Nen$_4$]. For further details on the history the reader is referred to Section 1.1. We give a formulation and a proof of the time-adiabatic theorem, which is maybe not the most concise one, but is best suited for a generalization to the space-adiabatic setting.

Theorem 2.2. *Let $H(t)$ satisfy the assumptions of Proposition 2.1 with $H(\cdot) \in C^2_{\mathrm{b}}(J, \mathcal{L}(\mathcal{D}, \mathcal{H}))$. Let $\sigma_*(t) \subset \sigma(H(t))$ satisfy the gap condition (1.5) on $J \subset \mathbb{R}$. Then $P_*(\cdot) \in C^2_{\mathrm{b}}(J, \mathcal{L}(\mathcal{H}))$ and there is a constant $C < \infty$ such that for $t, t_0 \in J$*

$$\| U^\varepsilon(t, t_0) - U^\varepsilon_{\mathrm{a}}(t, t_0) \| \leq C\,\varepsilon\,(1 + |t - t_0|)\,. \tag{2.1}$$

Here $U^\varepsilon_{\mathrm{a}}$ is the unitary propagator solving (1.8) on $\mathcal{D}$ with $H_{\mathrm{a}}(t)$ given through (1.7).
The right hand side of (2.1) can be replaced by

$$\varepsilon \left(\| F(t) \| + \| F(t_0) \| + \left| \int_{t_0}^{t} \mathrm{d}s\, \left(\| \dot{F}(s) \| + \| F(s)\,[\dot{P}(s),\, P(s)] \| \right) \right| \right)\,, \tag{2.2}$$

where $F(t)$ is defined in (2.10).

It is also worthwhile to give a more explicit bound in Theorem 2.2 than (2.2) for the simple case of an isolated eigenvalue.

Corollary 2.3. *Let $H(\cdot) \in C^2_{\mathrm{b}}(J, \mathcal{L}(\mathcal{H}))$ and $\sigma_*(t) = \{E(t)\}$ be an isolated eigenvalue. Denote by $\Delta(t)$ the size of the gap, i.e.*

$$\Delta(t) = \mathrm{dist}(E(t), \sigma(H(t)) \setminus E(t))\,.$$

Then (2.1) holds with the right hand side replaced by

$$2\,\varepsilon\left(\frac{\|\dot P(t)\|}{\Delta(t)}+\frac{\|\dot P(t_0)\|}{\Delta(t_0)}+\right.\\ \left.+\left|\int_{t_0}^{t}\mathrm{d}s\left(\frac{2\|\dot P(s)\|^2}{\Delta(s)}+\frac{\|\ddot P(s)\|}{\Delta(s)}+\frac{\|\dot P(s)\|\,\|\dot H(s)\|}{\Delta(s)^2}\right)\right|\right)\,. \tag{2.3}$$

The special form of the bound in Corollary 2.3 is clearly not optimal. However, it nicely displays the two mechanisms responsible for adiabatic decoupling. The size of the error depends on the size of the gap *and* on the variation of the eigenspaces. If either the gap is too small or the variation of the eigenspaces is too large, then adiabatic decoupling breaks down. On the other hand, if the eigenspaces are constant and only the eigenvalue varies, the subspaces decouple exactly. Moreover the rough estimate (2.3) suffices to prove the correct order of the non-adiabatic transitions near a regular eigenvalue crossing, cf. Corollary 2.5.

Proof (of Theorem 2.2). As the first step we show how the regularity of the spectral projection $P_*(t)$ as a function of t follows from the regularity of $H(t)$ and the gap condition. The argument is standard, cf. [Ka$_1$], and uses Riesz' formula,

$$P_*(t)=\frac{\mathrm{i}}{2\pi}\oint_{\Gamma(t)}\mathrm{d}\zeta\,\big(H(t)-\zeta\big)^{-1}\,. \tag{2.4}$$

Here $\Gamma(t)\subset\mathbb{C}$ is a positively oriented closed curve encircling $\sigma_*(t)$ once such that

$$\inf_{t\in J}\operatorname{dist}\big(\Gamma(t),\sigma(H(t))\big)=g/2\,.$$

Such a family of contours $\Gamma(t)$ exists because of the gap condition (1.5). Because of the continuity of the functions $f_\pm$ in (1.5), for each $\tau\in J$ there exists a neighborhood $I(\tau)$ of τ such that

$$\inf_{t\in I(\tau)}\operatorname{dist}\big(\Gamma(\tau),\sigma(H(t))\big)\geq g/4\,.$$

Hence for $t\in I(\tau)$ one obtains the representation

$$P_*(t)=\frac{\mathrm{i}}{2\pi}\oint_{\Gamma(\tau)}\mathrm{d}\zeta\,\big(H(t)-\zeta\big)^{-1}\,, \tag{2.5}$$

and it is now easy to differentiate (2.5) with respect to t. We find that for $t\in I(\tau)$

$$\frac{\mathrm{d}^n}{\mathrm{d}t^n}P_*(t)=\frac{\mathrm{i}}{2\pi}\oint_{\Gamma(\tau)}\mathrm{d}\zeta\,\frac{\mathrm{d}^n}{\mathrm{d}t^n}\big(H(t)-\zeta\big)^{-1} \tag{2.6}$$

whenever $R(\zeta,t):=(H(t)-\zeta)^{-1}\in C^n_{\mathrm{b}}(J,\mathcal{L}(\mathcal{H}))$.

Lemma 2.4. *Let $H(t) \in C^n_{\rm b}(I, \mathcal{L}(\mathcal{D}, \mathcal{H}))$ for some open interval $I \subset J$. Then $R(\zeta, \cdot) \in C^n_{\rm b}(I, \mathcal{L}(\mathcal{H}, \mathcal{D}))$ for all $\zeta \in \mathbb{C} \setminus \overline{\cup_{t\in I}\sigma(H(t))}$.*

Proof. First note that $R(\zeta, t) \in \mathcal{L}(\mathcal{H}, \mathcal{D})$ for $t \in I$ and thus

$$R(\zeta, t) - R(\zeta, s) = R(\zeta, t)\big(H(s) - H(t)\big)R(\zeta, s)$$

implies together with the assumption $H(t) \in C_{\rm b}(I, \mathcal{L}(\mathcal{D}, \mathcal{H}))$ that $R(\zeta, \cdot) \in C_{\rm b}(I, \mathcal{L}(\mathcal{H}, \mathcal{D}))$.

As for differentiability, one obtains from differentiating the identity

$$\mathbf{1} = (H(t) - \zeta)\, R(\zeta, t)$$

with respect to t that

$$\dot{R}(\zeta, t) = -R(\zeta, t)\, \dot{H}(t)\, R(\zeta, t)\,.$$

Hence $H(t) \in C^n_{\rm b}(I, \mathcal{L}(\mathcal{D}, \mathcal{H}))$ together with $R(\zeta, \cdot) \in C_{\rm b}(I, \mathcal{L}(\mathcal{H}, \mathcal{D}))$ implies that $R(\zeta, t) \in C^n_{\rm b}(I, \mathcal{L}(\mathcal{H}, \mathcal{D}))$. □

For $n = 2$ the claimed regularity of $P_*(t)$ follows from Lemma 2.4. Note also that $P_*(\cdot) \in C^2_{\rm b}(J, \mathcal{L}(\mathcal{H}))$ implies that $H^\varepsilon_{\rm a}(t)$ satisfies the assumptions of Proposition 2.1 as well and hence $U^\varepsilon_{\rm a}$ defines a propagator on $\mathcal{D}$.

We now turn to (2.1). Using the standard Cook's type argument one expresses the difference of the unitaries in terms of the difference of the generators,

$$\begin{aligned} U^\varepsilon(t, t_0) - U^\varepsilon_{\rm a}(t, t_0) &= -\,U^\varepsilon(t, t_0) \int_{t_0}^t {\rm d}t'\, \frac{\rm d}{{\rm d}t'}\Big(U^\varepsilon(t_0, t')\, U^\varepsilon_{\rm a}(t', t_0)\Big) \qquad (2.7)\\ &= -\frac{\rm i}{\varepsilon}\, U^\varepsilon(t, t_0) \int_{t_0}^t {\rm d}t'\, U^\varepsilon(t_0, t') \,\big(\, H(t') - H_{\rm a}(t')\,\big)\, U^\varepsilon_{\rm a}(t', t_0)\\ &= -\,U^\varepsilon(t, t_0) \int_{t_0}^t {\rm d}t'\, U^\varepsilon(t_0, t')\, [\dot{P}_*(t'), P_*(t')]\, U^\varepsilon_{\rm a}(t', t_0)\,. \end{aligned}$$

In (2.7) one uses that both propagators are strongly differentiable on $\mathcal{D}$ and that $U^\varepsilon_{\rm a}(t, t_0)\mathcal{D} = \mathcal{D}$ for all $t, t_0 \in J$. Although the difference of the generators $H(t) - H_{\rm a}(t) = {\rm i}\,\varepsilon\,[\dot{P}_*(t), P_*(t)]$ is of order ε, on first glance (2.7) suggests that this difference might add up to a difference of order 1 on the macroscopic time-scale. The key observation for adiabatic theory is that the integrand in (2.7) oscillates and can be written as the time-derivative of a function which is of order ε. In principle the situation is the same as for the function ${\rm e}^{{\rm i}t/\varepsilon}$, which is $\mathcal{O}(1)$, but integrated yields

$$\int_{t_0}^t {\rm d}t'\, {\rm e}^{{\rm i}t'/\varepsilon} = -{\rm i}\varepsilon\, \Big({\rm e}^{{\rm i}t_0/\varepsilon} - {\rm e}^{{\rm i}t/\varepsilon}\Big) = \mathcal{O}(\varepsilon)\,.$$

In order to motivate the following definition, consider for the moment the special case when $\sigma_*(t) = \{E(t)\}$ consists of a single eigenvalue $E(t)$. Then

$$F(t) = -\Big(R(E(t),t)\,\dot{P}_*(t)\,P_*(t) + P_*(t)\,\dot{P}_*(t)\,R(E(t),t)\Big) \tag{2.8}$$

obviously satisfies

$$[H(t), F(t)] = [\dot{P}_*(t), P_*(t)]\,. \tag{2.9}$$

Note that, in view of (1.15), $R(E(t),t)$ acts in (2.8) only on $P_*^\perp(t)\mathcal{H}$, where, as a consequence of the gap condition, it is bounded uniformly. Equation (2.9) shows that one part of the integrand in (2.7) can be written as a commutator of $F(t)$ with $H(t)$ and thus, at least approximately, as the time-derivative of $-\mathrm{i}\,\varepsilon\,U^\varepsilon(t_0,t)\,F(t)\,U^\varepsilon(t,t_0)$.

Generalizing (2.8) to the case of arbitrary $\sigma_*(t)$ one defines

$$F(t) = \frac{1}{2\pi\mathrm{i}} \oint_{\Gamma(t)} \mathrm{d}\zeta\, P_*^\perp(t)\,R(\zeta,t)\,\dot{R}(\zeta,t) + \mathrm{adj.} \tag{2.10}$$

where here and in the following "±adj." means that the adjoint of the sum of all operators to the left is added resp. subtracted. Using $H(t)R(\zeta,t) = \mathbf{1} + \zeta R(\zeta,t)$ and $\dot{R}(\zeta,t)\,(H(t)-\zeta) = -R(\zeta,t)\,\dot{H}(t)$, one computes

$$\begin{aligned}
[H(t), F(t)] &= \frac{1}{2\pi\mathrm{i}} \oint_{\Gamma(t)} \mathrm{d}\zeta\, \big[H(t), P_*^\perp(t)\,R(\zeta,t)\,\dot{R}(\zeta,t)\big] - \mathrm{adj.} \\
&= \frac{1}{2\pi\mathrm{i}} \oint_{\Gamma(t)} \mathrm{d}\zeta\, P_*^\perp(t)\,\Big(\big(\mathbf{1}+\zeta R(\zeta,t)\big)\,\dot{R}(\zeta,t) - R(\zeta,t)\,\dot{R}(\zeta,t)\,H(t)\Big) - \mathrm{adj.} \\
&= P_*^\perp(t)\,\dot{P}_*(t) - \frac{1}{2\pi\mathrm{i}} \oint_{\Gamma(t)} \mathrm{d}\zeta\, P_*^\perp(t)\,R(\zeta,t)\,\dot{R}(\zeta,t)\,(H(t)-\zeta) - \mathrm{adj.} \\
&= P_*^\perp(t)\,\dot{P}_*(t) + \frac{1}{2\pi\mathrm{i}} \oint_{\Gamma(t)} \mathrm{d}\zeta\, P_*^\perp(t)\,R^2(\zeta,t)\,\dot{H}(t) - \mathrm{adj.} \\
&= P_*^\perp(t)\,\dot{P}_*(t) - \mathrm{adj.} = [\dot{P}_*(t), P_*(t)]\,.
\end{aligned} \tag{2.11}$$

In the second to last equality of (2.11) we used that $\zeta \mapsto P_*^\perp(t)\,R^2(\zeta,t)$ is holomorphic inside of $\Gamma(t)$ and the last equality is a consequence of (1.15).

Now let

$$A(t) = -\mathrm{i}\,\varepsilon\,U^\varepsilon(t_0,t)\,F(t)\,U^\varepsilon(t,t_0)\,.$$

Since $P_*(\cdot) \in C_\mathrm{b}^2(\mathbb{R}, \mathcal{L}(\mathcal{H}))$ it follows that $F(\cdot) \in C_\mathrm{b}^1(\mathbb{R}, \mathcal{L}(\mathcal{H}))$ and thus

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}A(t) &= U^\varepsilon(t_0,t)\,[H(t), F(t)]\,U^\varepsilon(t,t_0) - \mathrm{i}\,\varepsilon\,U^\varepsilon(t_0,t)\,\dot{F}(t)\,U^\varepsilon(t,t_0) \\
&= U^\varepsilon(t_0,t)\,[\dot{P}_*(t), P_*(t)]\,U^\varepsilon(t,t_0) + \mathcal{O}(\varepsilon)\,.
\end{aligned} \tag{2.12}$$

Finally we insert (2.12) into (2.7) and integrate by parts,

$$
\begin{aligned}
&\left\| U^\varepsilon(t,t_0) - U_{\mathrm{a}}^\varepsilon(t,t_0) \right\| \leq \\
&\quad \leq \left\| \int_{t_0}^t \mathrm{d}t' \, \left(\frac{\mathrm{d}}{\mathrm{d}t'} A(t') \right) U^\varepsilon(t_0,t') \, U_{\mathrm{a}}^\varepsilon(t',t_0) \right\| + \varepsilon \, |t-t_0| \sup_{s\in[t_0,t]} \|\dot{F}(s)\| \\
&\quad \leq \|A(t)\| + \|A(t_0)\| \\
&\qquad + \left\| \int_{t_0}^t \mathrm{d}t' \, A(t') \left(\frac{\mathrm{d}}{\mathrm{d}t'} \, U^\varepsilon(t_0,t') \, U_{\mathrm{a}}^\varepsilon(t',t_0) \right) \right\| + \mathcal{O}(\varepsilon|t-t_0|) \\
&\quad = \mathcal{O}(\varepsilon(1+|t-t_0|)) \,. \qquad (2.13)
\end{aligned}
$$

In (2.13) it was used that $\|A(t)\| = \mathcal{O}(\varepsilon)$ uniformly for $t \in \mathbb{R}$ and that $\|\frac{\mathrm{d}}{\mathrm{d}t'} U^\varepsilon(t_0,t') \, U_{\mathrm{a}}^\varepsilon(t',t_0)\| = \|U^\varepsilon(t_0,t') \, [\dot{P}_*(t'), P_*(t')] \, U_{\mathrm{a}}^\varepsilon(t',t_0)\|$ is uniformly bounded.

The explicit bound (2.2) follows immediately from an examination of the above argument. □

We end this section with a simple corollary, which handles the case of regular eigenvalue crossings. Consider again the situation of Theorem 2.2, but with $\sigma_*(t) = \{E_1(t), E_2(t)\}$ consisting of two eigenvalues of $H(t)$, $H(\cdot) \in C_{\mathrm{b}}^n(J, \mathcal{L}(\mathcal{H}))$. Assume that on the relevant time-interval $J \subset \mathbb{R}$ we have

$$
E_1(t) = E_2(t) \qquad \Leftrightarrow \qquad t = t_{\mathrm{c}} \in J \,,
$$

i.e. the eigenvalues cross exactly once at t_{c}. The labelling of $E_1(t)$ and $E_2(t)$ is such that $E_1(t)$ and $E_2(t)$ are in $C_{\mathrm{b}}^n(J, \mathbb{R})$, cf. Figure 2.1. Furthermore we assume that the corresponding spectral projections $P_1(t)$ and $P_2(t)$ can be continued smoothly across the point t_{c} and are thus in $C_{\mathrm{b}}^n(J, \mathcal{L}(\mathcal{H}))$. The adiabatic Hamiltonian is now defined as

$$
H_{\mathrm{a}}(t) = H(t) - \mathrm{i}\,\varepsilon \, P_1(t) \, \dot{P}_1(t) - \mathrm{i}\,\varepsilon \, P_2(t) \, \dot{P}_2(t) - \mathrm{i}\,\varepsilon \, P_*^\perp(t) \, \dot{P}_*^\perp(t) \,,
$$

where $P_*^\perp(t) = \mathbf{1} - P_1(t) - P_2(t)$.

Corollary 2.5. *Let $H(\cdot) \in C_{\mathrm{b}}^n(J, \mathcal{L}(\mathcal{H}))$, $n \geq 2$, and $\sigma_*(t) = \{E_1(t), E_2(t)\}$ be as above. If*

$$
\partial_t^k \, \big(E_1(t) - E_2(t)\big)|_{t=t_{\mathrm{c}}} \neq 0 \quad \textit{for some} \quad 1 \leq k \leq n \,,
$$

then there is a constant $C < \infty$ such that for all $t, t_0 \in J \setminus \{t_{\mathrm{c}}\}$

$$
\| \, U^\varepsilon(t,t_0) - U_{\mathrm{a}}^\varepsilon(t,t_0) \| \leq C \, \varepsilon^{1/(2k)} \, (1 + |t-t_0|) \,. \qquad (2.14)
$$

Proof. The only new situation occurs when the crossing time t_{c} lies between t and t_0. Without restricting generality we can assume that $t_0 < t_{\mathrm{c}} < t$. Splitting the time interval into the region near the crossing and away from it, we obtain

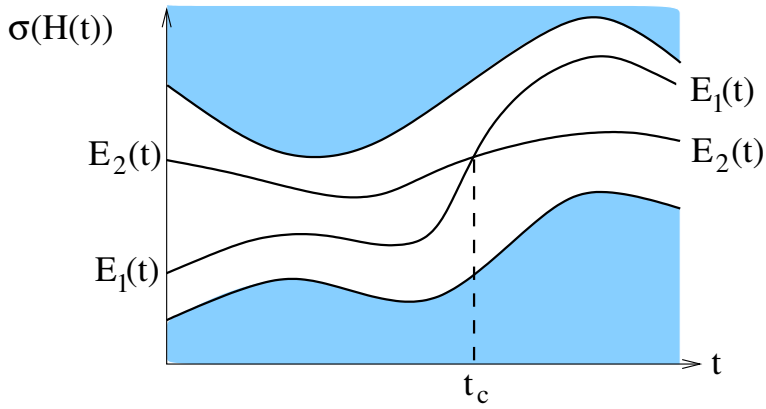

Fig. 2.1. Linear crossing of eigenvalues.

$$\begin{aligned}\| U^\varepsilon(t,t_0) - U_{\mathrm{a}}^\varepsilon(t,t_0) \| &\le \| U^\varepsilon(t_{\mathrm{c}} - \varepsilon^{1/(2k)}, t_0) - U_{\mathrm{a}}^\varepsilon(t_{\mathrm{c}} - \varepsilon^{1/(2k)}, t_0) \| \\ &+ \| U^\varepsilon(t_{\mathrm{c}} + \varepsilon^{1/(2k)}, t_{\mathrm{c}} - \varepsilon^{1/(2k)}) - U_{\mathrm{a}}^\varepsilon(t_{\mathrm{c}} + \varepsilon^{1/(2k)}, t_{\mathrm{c}} - \varepsilon^{1/(2k)}) \| \\ &+ \| U^\varepsilon(t, t_{\mathrm{c}} + \varepsilon^{1/(2k)}) - U_{\mathrm{a}}^\varepsilon(t, t_{\mathrm{c}} + \varepsilon^{1/(2k)}) \| . \end{aligned} \tag{2.15}$$

Since we have that $P_1(\cdot)$ and $P_2(\cdot)$ are in $C_{\mathrm{b}}^n(J, \mathcal{L}(\mathcal{H}))$, away from the crossing the order of the error is completely determined by the size of the gap $\Delta(s) = |E_1(s) - E_2(s)|$ as in (2.3). Taylor expansion near t_{c} yields that $\Delta(s) \ge C\,|s - t_c|^k$ and thus the first term in (2.15) (and analogously the last one) can be bounded as

$$\begin{aligned}&\| U^\varepsilon(t_{\mathrm{c}} - \varepsilon^{1/(2k)}, t_0) - U_{\mathrm{a}}^\varepsilon(t_{\mathrm{c}} - \varepsilon^{1/(2k)}, t_0) \| \\ &\quad \le C\,\varepsilon \left(1 + \varepsilon^{-1/(2k)} + \varepsilon^{(-k+1)/(2k)} + \varepsilon^{(-2k+1)/(2k)} \right) \le \widetilde{C}\,\varepsilon^{1/(2k)} . \end{aligned}$$

The remaining term in (2.15) can be bounded by rewriting it as in (2.7) and using that the integrand is bounded and that the domain of integration is of order $\varepsilon^{1/(2k)}$. □

2.2 Perturbations of fibered Hamiltonians

One can think of $\mathrm{i}\varepsilon\partial_t$ as a perturbation of the family $H(t)$ of self-adjoint operators: the spectral subspaces of $H(t)$ are not invariant under time-evolution because the commutator $[\mathrm{i}\varepsilon\partial_t, H(t)] \neq 0$ does not vanish. However, for small ε the commutator is small and one can show that spectral subspaces corresponding to spectrum which is separated by a gap are approximately invariant.

It turns out that one can generalize the proof of Theorem 2.2 in a straightforward way to the case where $H_0(x)$ is a family of self-adjoint operators on

some Hilbert space $\mathcal{H}_{\rm f}$ depending on the parameter $x \in \mathbb{R}^d$ and the Hamiltonian is given through

$$H^\varepsilon = f(-\mathrm{i}\varepsilon\nabla_x) \otimes \mathbf{1} + \int_{\mathbb{R}^d}^{\oplus} \mathrm{d}x\, H_0(x)\,. \tag{2.16}$$

The Hamiltonian H^ε now acts on $\mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathcal{H}_{\rm f} = L^2(\mathbb{R}^d, \mathcal{H}_{\rm f})$ and $f(-\mathrm{i}\varepsilon\nabla_x)$ with $f : \mathbb{R}^d \to \mathbb{R}$ is the perturbation which in a sense replaces $\mathrm{i}\varepsilon\partial_t$.

In physical applications the splitting of the Hilbert space corresponds to the splitting of the system into *slow* and *fast* degrees of freedom. The Hilbert space for the fast degrees of freedom is $\mathcal{H}_{\rm f}$ and its explicit form is irrelevant for the following analysis. The Hilbert space for the slow degrees of freedom is $L^2(\mathbb{R}^d)$, or, more general, the L^2 space over some other configuration space. While the identification of slow and fast degrees of freedom is obvious in some cases, as e.g. in molecular dynamics, where the nuclei move slowly compared to the electrons, in other cases some analysis of the problem is required to cast a given Hamiltonian into the form (2.16), cf. [HST, TeSp].

Remark 2.6. Recall that a self-adjoint operator H acting on the Hilbert space

$$L^2(\mathbb{R}^d) \otimes \mathcal{H}_{\rm f} = \int_{\mathbb{R}^d}^{\oplus} \mathrm{d}x\, \mathcal{H}_{\rm f}$$

is called fibered, cf. [ReSi$_4$], if there is a family $H(x)$, $x \in \mathbb{R}^d$, of self-adjoint operators on $\mathcal{H}_{\rm f}$, such that the map $x \mapsto \langle \psi, \big(H(x) - \mathrm{i}\big)^{-1}\phi\rangle$ is measurable for all $\psi, \phi \in \mathcal{H}_{\rm f}$ and such that

$$(H - \mathrm{i})^{-1} = \int_{\mathbb{R}^d}^{\oplus} \mathrm{d}x\, \big(H(x) - \mathrm{i}\big)^{-1}\,.$$

In this case one writes

$$H = \int_{\mathbb{R}^d}^{\oplus} \mathrm{d}x\, H(x)\,.$$

For a detailed and careful discussion of fibered operators see also the Appendix of [Hoe]. ♢

We will call the set

$$\Sigma = \big\{(x,s) \in \mathbb{R}^d \times \mathbb{R} : s \in \sigma(H_0(x))\big\}$$

the *fibered spectrum* of H_0. In the following conditions on the regularity of $H_0(\cdot)$ will be imposed, which ensure that Σ is defined without ambiguities about null sets.

Let $\sigma_* \subset \Sigma$ be such that $x \mapsto P_*(x)$ is measurable, where $P_*(x)$ denotes the spectral projection of $H_0(x)$ associated with $\sigma_*(x)$. Then $P_* =$

$\int_{\mathbb{R}^d} \mathrm{d}x\, P_*(x)$ is an orthogonal projection which commutes with H_0, but which is, in general, not a spectral projection of H_0. In particular, the subspace $P_*\mathcal{H}$ is an invariant subspace for the dynamics generated by H_0,

$$\big[\, \mathrm{e}^{-\mathrm{i}H_0 s},\, P_* \,\big] = 0\,.$$

We think of (2.16) as "small" perturbation of a fibered Hamiltonian. The perturbation $f(-\mathrm{i}\varepsilon\nabla_x) \otimes \mathbf{1}$ is small in the sense that now

$$[\, H^\varepsilon,\, P_* \,] = [\, f(-\mathrm{i}\varepsilon\nabla_x) \otimes \mathbf{1},\, P_* \,] = \mathcal{O}(\varepsilon)$$

and thus the subspaces $P_*\mathcal{H}$ are at least approximately invariant for small ε,

$$\Big[\, \mathrm{e}^{-\mathrm{i}H^\varepsilon s},\, P_* \,\Big] = \mathcal{O}(\varepsilon\,|s|)\,. \tag{2.17}$$

However, as we saw in the example of Section 1.2.1, one is interested in the dynamics for finite *macroscopic* times $t = \varepsilon s$. For macroscopic times the naive argument leading to (2.17) gives

$$\Big[\, \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon},\, P_* \,\Big] = \mathcal{O}(|t|)\,, \tag{2.18}$$

which does not become small with small ε.

The situation is exactly as in the time-adiabatic case, where the naive argument yields (2.7), which is of order $\mathcal{O}(1)$ at first glance. And indeed, one can use exactly the same line of arguments as in the time-adiabatic case in order to improve (2.18) to

$$\Big[\, \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon},\, P_* \,\Big] = \mathcal{O}(\varepsilon(1 + |t|))$$

if $\sigma_*(x)$ is separated by a gap from the remainder of the spectrum of $H_0(x)$ uniformly for $x \in \mathbb{R}^d$. More precisely we assume that the spectrum $\sigma(x)$ of $H_0(x)$ contains a subset $\sigma_*(x) \subset \sigma(x)$ such that there are real-valued functions $f_\pm \in C_\mathrm{b}(\mathbb{R}^d)$ defining an interval $I(x) = [f_-(x), f_+(x)]$ with

$$\sigma_*(x) \subset I(x) \quad \text{and} \quad \inf_{x\in\mathbb{R}^d} \mathrm{dist}\big(I(x), \sigma(x) \setminus \sigma_*(x)\big) =: g > 0\,. \tag{2.19}$$

In the space-adiabatic setting the adiabatic evolution is generated by the diagonal Hamiltonian

$$H^\varepsilon_\mathrm{diag} = P_*\, H^\varepsilon\, P_* + P_*^\perp\, H^\varepsilon\, P_*^\perp\,,$$

which by construction satisfies

$$\Big[\, \mathrm{e}^{-\mathrm{i}H^\varepsilon_\mathrm{diag} t/\varepsilon},\, P_* \,\Big] = 0\,.$$

We illustrate the general scheme under simplifying and rather restrictive assumptions. In Section 2.3 we apply the same scheme to molecular dynamics and prove the time-dependent Born-Oppenheimer approximation. The general scheme is reconsidered in Chapter 6 under less restrictive assumptions and, in particular, without assuming a gap condition.

Theorem 2.7. *Let $H_0(x)$, $x \in \mathbb{R}^d$, be a family of bounded self-adjoint operators such that $H_0(\cdot) \in C^2_{\rm b}(\mathbb{R}^d, \mathcal{L}(\mathcal{H}_{\rm f}))$ and let $\sigma_*(x) \subset \sigma(x)$ satisfy the gap condition (2.19). Let $f \in \mathcal{S}(\mathbb{R}^d)$ be real-valued and H^ε be the bounded self-adjoint operator on $\mathcal{H} = L^2(\mathbb{R}^d, \mathcal{H}_{\rm f})$ given through (2.16). Then there is a constant $C < \infty$ such that for all $t \in \mathbb{R}$*

$$\left\| \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} - \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm diag} t/\varepsilon} \right\|_{\mathcal{L}(\mathcal{H})} \leq C\,\varepsilon\,(1+|t|)\,. \tag{2.20}$$

Proof. From the general argument presented in the the proof of Theorem 2.2 it follows that $P_*(\cdot) \in C^2_{\rm b}(\mathbb{R}^d, \mathcal{L}(\mathcal{H}))$ and as in (2.7) we find that

$$\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} - \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm diag} t/\varepsilon} = -\frac{\mathrm{i}}{\varepsilon}\,\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} \int_0^t \mathrm{d}t'\,\mathrm{e}^{\mathrm{i}H^\varepsilon t'/\varepsilon}\,H^\varepsilon_{\rm od}\,\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm diag} t'/\varepsilon}\,. \tag{2.21}$$

The off-diagonal part of the Hamiltonian is defined as

$$\begin{aligned} H^\varepsilon_{\rm od} &:= H^\varepsilon - H^\varepsilon_{\rm diag} = P_*^\perp \left(f(-\mathrm{i}\varepsilon\nabla_x) \otimes \mathbf{1}_{\mathcal{H}_{\rm f}} \right) P_* + \text{adj.} \\ &= P_*^\perp \left[\left(f(-\mathrm{i}\varepsilon\nabla_x) \otimes \mathbf{1}_{\mathcal{H}_{\rm f}} \right),\, P_* \right] P_* + \text{adj.}\,. \end{aligned}$$

Here and in the following "± adj." means that the adjoint operator of all the operators to the left in an expression are added resp. subtracted. While in the time-adiabatic case we obtained the simple expression $[-\mathrm{i}\varepsilon\partial_t, P_*] = -\mathrm{i}\varepsilon\dot{P}_*$, now the commutator gives an analogous expression, however, with a remainder term of order $\mathcal{O}(\varepsilon^2)$.

Lemma 2.8. *Let $g \in \mathcal{S}(\mathbb{R}^d)$ and $A(\cdot) \in C^n_{\rm b}(\mathbb{R}^d, \mathcal{L}(\mathcal{H}_{\rm f}))$ and let $g^\varepsilon := g(-\mathrm{i}\varepsilon\nabla_x) \otimes \mathbf{1}_{\mathcal{H}_{\rm f}}$.*

(i) *If $n = 1$, then $[\,g^\varepsilon,\, A\,] = \mathcal{O}(\varepsilon)$.*
(ii) *If $n \geq 2$, then $[\,g^\varepsilon,\, A\,] = -\mathrm{i}\,\varepsilon\,(\nabla A)\cdot(\nabla g)^\varepsilon + \mathcal{O}(\varepsilon^2)$.*

Here the errors hold in the norm of $\mathcal{L}(\mathcal{H})$, $\nabla A = \int_{\mathbb{R}^d}^{\oplus} \mathrm{d}x\,\nabla A(x)$ and $(\nabla g)^\varepsilon = (\nabla g)(-\mathrm{i}\varepsilon\nabla_x) \otimes \mathbf{1}_{\mathcal{H}_{\rm f}}$.

Proof. Using Taylor expansion with rest we find that for $n \geq 2$

$$\begin{aligned} A(x-\varepsilon y) \;&=\; A(x) - \varepsilon\, y\cdot\nabla A(x) + \varepsilon^2 \int_0^1 \mathrm{d}\eta\,\langle\, y,\, \nabla^{(2)} A(x-\eta\varepsilon y)\, y\,\rangle_{\mathbb{R}^d} \\ &=: A(x) - \varepsilon\, y\cdot\nabla A(x) + \varepsilon^2\, R^\varepsilon(x,y)\,, \end{aligned}$$

where $\nabla^{(2)}A$ denotes the Hessian and $\|R^\varepsilon(x,y)\|_{\mathcal{L}(\mathcal{H}_{\rm f})} = \mathcal{O}(|y|^2)$. Hence we find for $\psi \in \mathcal{H}$ that

$$\begin{aligned} \big(g^\varepsilon A\,\psi\big)(x) &= ((2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} \mathrm{d}y\,\widehat{g}(y)\,A(x-\varepsilon y)\,\psi(x-\varepsilon y) \\ &= (2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} \mathrm{d}y\,\widehat{g}(y)\,\big(A(x) - \varepsilon\, y\cdot(\nabla A)(x) + R^\varepsilon(x,y)\big)\,\psi(x-\varepsilon y) \\ &= \big(A\,g^\varepsilon\,\psi\big)(x) - \mathrm{i}\,\varepsilon\,\big((\nabla A)\cdot(\nabla g)^\varepsilon\,\psi\big)(x) + \varepsilon^2\,\big(R^\varepsilon\,\psi\big)(x)\,, \end{aligned}$$

where $\|R^\varepsilon\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(1)$. This implies (ii). Stopping the Taylor expansion at first order for $n = 1$, one obtains (i). □

Since $P_*(\cdot) \in C^2_{\mathrm{b}}(\mathbb{R}^d, \mathcal{L}(\mathcal{H}_{\mathrm{f}}))$, the Lemma implies that

$$[\, f^\varepsilon,\, P_* \,] = -\mathrm{i}\,\varepsilon\,(\nabla P_*)\cdot(\nabla f)^\varepsilon + \mathcal{O}(\varepsilon^2)$$

and thus

$$\begin{aligned} H^\varepsilon_{\mathrm{od}} &= -\mathrm{i}\,\varepsilon\, P_*^\perp\,(\nabla P_*)\cdot(\nabla f)^\varepsilon\, P_* + \mathrm{adj.} + \mathcal{O}(\varepsilon^2) \\ &= -\mathrm{i}\,\varepsilon\, P_*^\perp\,(\nabla P_*)\, P_*\cdot(\nabla f)^\varepsilon + \mathrm{adj.} + \mathcal{O}(\varepsilon^2)\,. \end{aligned} \tag{2.22}$$

For the last equality we used again Lemma 2.8 to commute $(\nabla f)^\varepsilon$ through P_* Since clearly (1.15) generalizes to

$$\nabla P_* = P_*^\perp\,(\nabla P_*)\, P_* + P_*\,(\nabla P_*)\, P_*^\perp\,,$$

we define in analogy to (2.10), but without the adjoint term for the moment,

$$F(x) = \frac{1}{2\pi\mathrm{i}} \oint_{\Gamma(x)} \mathrm{d}\zeta\, P_*^\perp(x)\, R(\zeta, x)\, (\nabla R)(\zeta, x)\,. \tag{2.23}$$

As in (2.11) one concludes that

$$[\, H_0(x),\, F(x)\,] = (\nabla P_*)(x)\, P_*(x)\,.$$

Let

$$G = F\cdot(\nabla f)^\varepsilon + \mathrm{adj.}\,,$$

then $F(\cdot) \in C^1_{\mathrm{b}}(\mathbb{R}^d, \mathcal{L}(\mathcal{H}_{\mathrm{f}})^{\oplus d})$ and Lemma (2.8) (i) yield

$$\begin{aligned} [\, H^\varepsilon,\, G\,] &= [\, f^\varepsilon,\, F\,]\cdot(\nabla f)^\varepsilon + [\, H_0,\, F\,]\cdot(\nabla f)^\varepsilon + F\cdot[\, H^\varepsilon,\, (\nabla f)^\varepsilon\,] - \mathrm{adj.} \\ &= (\nabla P_*)\, P_*\cdot(\nabla f)^\varepsilon - \mathrm{adj.} + \mathcal{O}(\varepsilon)\,. \end{aligned}$$

As in the time-adiabatic case we define

$$A(t) = -\mathrm{i}\,\varepsilon\, \mathrm{e}^{\mathrm{i}H^\varepsilon t/\varepsilon}\, G\, \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}\,,$$

such that

$$\frac{\mathrm{d}}{\mathrm{d}t}A(t) = \mathrm{e}^{\mathrm{i}H^\varepsilon t/\varepsilon}\,[\, H^\varepsilon,\, G\,]\,\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} = \frac{\mathrm{i}}{\varepsilon}\,\mathrm{e}^{\mathrm{i}H^\varepsilon t/\varepsilon}\, H^\varepsilon_{\mathrm{od}}\,\mathrm{e}^{-\mathrm{i}H^\varepsilon \frac{t}{\varepsilon}} + \mathcal{O}(\varepsilon)\,. \tag{2.24}$$

Finally we insert (2.24) into (2.21) and integrate by parts,

$$\begin{aligned} &\left\| \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} - \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{diag}} t/\varepsilon} \right\| = \\ &\quad = \left\| \int_0^t \mathrm{d}t' \left(\frac{\mathrm{d}}{\mathrm{d}t'} A(t') \right) \mathrm{e}^{\mathrm{i}H^\varepsilon t'/\varepsilon}\, \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{diag}} t'/\varepsilon} \right\| + \mathcal{O}(\varepsilon|t|) \\ &\quad \le \|A(t)\| + \|A(0)\| \\ &\qquad + \left\| \int_0^t \mathrm{d}t'\, A(t') \left(\frac{\mathrm{d}}{\mathrm{d}t'}\, \mathrm{e}^{\mathrm{i}H^\varepsilon t'/\varepsilon}\, \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{diag}} t'/\varepsilon} \right) \right\| + \mathcal{O}(\varepsilon|t|) \\ &\quad = \mathcal{O}(\varepsilon(1+|t|))\,. \end{aligned} \tag{2.25}$$

In (2.25) it was used that $\|A(t)\| = \mathcal{O}(\varepsilon)$ uniformly for $t \in \mathbb{R}$ and that

$$\left\| \frac{\mathrm{d}}{\mathrm{d}t'} \mathrm{e}^{\mathrm{i}H^\varepsilon t'/\varepsilon} \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{diag}} t'/\varepsilon} \right\| = \left\| \frac{\mathrm{i}}{\varepsilon} \mathrm{e}^{\mathrm{i}H^\varepsilon t'/\varepsilon} H^\varepsilon_{\mathrm{od}} \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{diag}} t'/\varepsilon} \right\|$$

is uniformly bounded according to (2.22). □

2.3 Time-dependent Born-Oppenheimer theory: Part I

The physical background of the time-dependent Born-Oppenheimer approximation was already discussed in the Introduction. In the present section we apply the first-order space-adiabatic scheme, which was developed in the previous section, to the full molecular Hamiltonian for l nuclei and k electrons:

$$\begin{aligned} H_{\mathrm{mol}} = \frac{1}{2m_{\mathrm{n}}} \sum_{n=1}^{l} \big(-\mathrm{i}\hbar\nabla_{x_n} + A(x_n)\big)^2 + \frac{1}{2m_{\mathrm{e}}} \sum_{n=1}^{k} \big(-\mathrm{i}\hbar\nabla_{y_n} - A(y_n)\big)^2 \\ + V_{\mathrm{e}}(y) + V_{\mathrm{en}}(x,y) + V_{\mathrm{n}}(x)\,. \end{aligned} \tag{2.26}$$

As compared to (1.30), we added the vector potential $A : \mathbb{R}^3 \to \mathbb{R}^3$ of an external magnetic field $B = \nabla \times A$. The electrons are modelled as point charges and the electronic repulsion is thus given through the Coulomb potential energy

$$V_{\mathrm{e}}(y) = \sum_{n=1}^{k-1} \sum_{m=n+1}^{k} \frac{1}{|y_n - y_m|}\,.$$

For technical and physical reasons, the nuclei are modelled as smeared rigid charge distributions $\rho \in C_0^\infty(\mathbb{R}^3)$, $\rho \geq 0$ and $\|\rho\|_{L^1} = 1$. As a consequence the potential for nuclear repulsion is

$$V_{\mathrm{n}}(x) = \sum_{n=1}^{l-1} \sum_{m=n+1}^{l} \int_{\mathbb{R}^6} \mathrm{d}z\, \mathrm{d}z'\, \frac{\rho(z - x_n)\rho(z' - x_m)}{|z - z'|}$$

and the attractive potential between electrons and nuclei is

$$V_{\mathrm{en}}(x,y) = -\sum_{n=1}^{l} \sum_{m=1}^{k} \int_{\mathbb{R}^3} \mathrm{d}z\, \frac{\rho(z - x_n)}{|z - y_m|}\,.$$

Note that V_{n} and V_{en} are bounded and the function $x \mapsto V_{\mathrm{en}}(x,\cdot) \in L^\infty$ is smooth.

As explained in Section 1.2.1, we change units such that $\hbar = m_{\mathrm{e}} = 1$, introduce $\varepsilon = \sqrt{m_{\mathrm{e}}/m_{\mathrm{n}}}$ and write

$$H^\varepsilon_{\mathrm{mol}} = \frac{\varepsilon^2}{2} \big(-\mathrm{i}\nabla_x + A(x)\big)^2 + \int_{\mathbb{R}^{3l}}^{\oplus} \mathrm{d}x\, H_{\mathrm{e}}(x)\,, \tag{2.27}$$

where

$$H_{\rm e}(x) = \frac{1}{2}\big(-{\rm i}\nabla_y - A(y)\big)^2 + V_{\rm e}(y) + V_{\rm en}(x,y) + V_{\rm n}(x) \tag{2.28}$$

is self-adjoint with x-independent domain $D(H_{\rm e}(x)) = H^2(\mathbb{R}^{3k}) \subset L^2(\mathbb{R}^{3k})$ under appropriate conditions on A. To simplify notation, we extended $A : \mathbb{R}^3 \to \mathbb{R}^3$ to $A : \mathbb{R}^{3l} \to \mathbb{R}^{3l}$ by repeating it l times.

The specific form (2.28) of the electronic part of the Hamiltonian will be of no importance in the following. As in the previous section we take some arbitrary separable Hilbert space $\mathcal{H}_{\rm e}$ for the electronic degrees of freedom. For the electronic Hamiltonian we only assume that

$$H_{\rm e} = \int_{\mathbb{R}^d}^{\oplus} {\rm d}x\, H_{\rm e}(x)\,, \qquad H_{\rm e}(x) = H_{\rm e0} + H_{\rm e1}(x)\,,$$

where $H_{\rm e0}$ is self-adjoint on some dense domain $\mathcal{D} \subset \mathcal{H}_{\rm e}$ and bounded from below and $H_{\rm e1}(x) \in \mathcal{L}(\mathcal{H}_{\rm e})$ is a continuous family of self-adjoint operators, bounded uniformly for $x \in \mathbb{R}^d$. Thus $H_{\rm e}$ is self-adjoint on $D(H_{\rm e}) = L^2(\mathbb{R}^d) \otimes \mathcal{D} \subset \mathcal{H} := L^2(\mathbb{R}^d) \otimes \mathcal{H}_{\rm e}$ and bounded from below. To properly define $L^2(\mathbb{R}^d) \otimes \mathcal{D}$ we equip $\mathcal{D}$ with the graph-norm $\|\cdot\|_{H_{\rm e0}}$, i.e., for $\psi \in \mathcal{D}$, $\|\psi\|_{H_{\rm e0}} = \|H_{\rm e0}\psi\| + \|\psi\|$.

Remark 2.9. Note that the general assumptions on $H_{\rm e}(x)$ allow one to include in addition to (2.28) also the spin of the electrons and relativistic corrections. ♢

Let $A \in C^1_{\rm b}(\mathbb{R}^d, \mathbb{R}^d)$. Then $\frac{\varepsilon^2}{2}\Big(-{\rm i}\nabla_x + A(x)\Big)^2$ is self-adjoint on $H^2(\mathbb{R}^d)$, the second Sobolev space, since $-{\rm i}\nabla_x$ is infinitesimally operator bounded with respect to $-\Delta_x$. It follows that

$$H^\varepsilon = \frac{\varepsilon^2}{2}\Big(-{\rm i}\nabla_x + A(x)\Big)^2 \otimes \mathbf{1}_{\mathcal{H}_{\rm e}} + H_{\rm e} \tag{2.29}$$

is self-adjoint on $D(H^\varepsilon) = H^2(\mathbb{R}^d) \otimes \mathcal{H}_{\rm e} \cap D(H_{\rm e})$.

In Section 2.2 we assumed for simplicity that the relevant part of the spectrum $\sigma_*(x)$ of the fibered Hamiltonian is separated by a gap for x in *all* of $\mathbb{R}^d$. However, in applications like in the present case, $H_{\rm e}(x)$ has isolated energy bands, in general, only locally in the configuration space of the nuclei, cf. Figure 2.2. In the following $\Lambda \subset \mathbb{R}^d$ denotes the region of configuration space of the nuclei that we are interested in. The local setting, $\Lambda \subset \mathbb{R}^d$, for the Born-Oppenheimer approximation will be discussed in Section 2.3.2, while Section 2.3.1 deals with the global case $\Lambda = \mathbb{R}^d$. We first treat the global case, since it allows us to consider arbitrary spectrum in $\sigma_*(x)$, e.g. $\sigma_*(x)$ could consist of a group of energy bands with crossings among the bands contained in $\sigma_*(x)$, cf. Figure 2.2.

For $x \in \Lambda$, $\Lambda \subset \mathbb{R}^d$ open, we require some regularity for $H_{\rm e}(x)$ as a function of x:

Condition $\mathbf{H}_k$. $H_{\rm e1}(\cdot) \in C^k_{\rm b}(\Lambda, \mathcal{L}(\mathcal{H}_{\rm e}))$.

The exact value of k will depend on whether $\Lambda = \mathbb{R}^d$ or $\Lambda \subset \mathbb{R}^d$. For the molecular Hamiltonian (2.26) with smeared nucleonic charge distribution, Condition $\mathbf{H}_k$ is easily checked and puts constraints only on the smoothness of the external potentials and on the smoothness and the decay of the charge distribution of the nuclei. For point nuclei $\mathbf{H}_k$ fails and a suitable substitute would require a generalization of the Hunziker distortion method of [KMSW].

We will be interested in subsets of the fibered spectrum of $H_{\rm e}$ which satisfy the local gap condition.

Condition (Gap on Λ). *For $x \in \Lambda$, let $\sigma_*(x) \subset \sigma(H_{\rm e}(x))$ be such that there are functions $f_\pm \in C_{\rm b}(\Lambda, \mathbb{R})$ defining an interval $I(x) = [f_-(x), f_+(x)]$ such that*

$$\sigma_*(x) \subset I(x) \quad \textit{and} \quad \inf_{x\in\Lambda} \operatorname{dist}\big(I(x), \sigma(H_{\rm e}(x)) \setminus \sigma_*(x)\big) =: g > 0.$$

As before, we set $P_* = \int_\Lambda^\oplus \mathrm{d}x\, P_*(x)$, where $P_*(x)$ is the spectral projection of $H_{\rm e}(x)$ with respect to $\sigma_*(x)$.

2.3.1 A global result

We assume $\Lambda = \mathbb{R}^d$ and let

$$H^\varepsilon_{\rm diag} := P_*\, H^\varepsilon\, P_* + P_*^\perp\, H^\varepsilon\, P_*^\perp\,. \tag{2.30}$$

Since we aim at a uniform result for the adiabatic theorem, cf. Remark 2.11, we introduce the Sobolev spaces $H^{1,\varepsilon}(\mathbb{R}^d)$ and $H^{2,\varepsilon}(\mathbb{R}^d)$ with respect to the ε-scaled gradient, i.e.

$$H^{1,\varepsilon}(\mathbb{R}^d) = \big\{\phi \in L^2(\mathbb{R}^d) : \|\phi\|^2_{H^{1,\varepsilon}} := \|\varepsilon\,|\nabla\phi|\,\|^2 + \|\phi\|^2 < \infty\big\}$$

and

$$H^{2,\varepsilon}(\mathbb{R}^d) = \big\{\phi \in L^2(\mathbb{R}^d) : \|\phi\|^2_{H^{2,\varepsilon}} := \|\varepsilon^2\Delta\phi\|^2 + \|\phi\|^2 < \infty\big\}\,.$$

Alternatively we will project on finite total energies and define $\mathcal{E}(H^\varepsilon) := \mathbf{1}_{(-\infty,\mathcal{E}]}(H^\varepsilon)$ as the projection on total energies smaller than $\mathcal{E}$.

Theorem 2.10. *Assume Condition $\mathbf{H}_3$ and Condition* **Gap** *for $\Lambda = \mathbb{R}^d$. Then $H^\varepsilon_{\rm diag}$ is self-adjoint on the domain of H^ε. There are constants $C, \widetilde{C} < \infty$ such that for all $t \in \mathbb{R}$*

$$\Big\| \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} - \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm diag} t/\varepsilon} \Big\|_{\mathcal{L}(H^{2,\varepsilon}\otimes\mathcal{H}_{\rm e},\mathcal{H})} \le \varepsilon\, C\,(1+|t|)^3 \tag{2.31}$$

and for all $\mathcal{E} \in \mathbb{R}$

$$\Big\| \Big(\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} - \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm diag} t/\varepsilon}\Big)\, \mathcal{E}(H^\varepsilon) \Big\|_{\mathcal{L}(\mathcal{H})} \le \varepsilon\, \widetilde{C}\,(1+|\mathcal{E}|)\,(1+|t|)\,. \tag{2.32}$$

$\mathcal{L}(H^{2,\varepsilon}\otimes\mathcal{H}_{\rm e},\mathcal{H})$ denotes the space of bounded linear operators from $H^{2,\varepsilon}\otimes\mathcal{H}_{\rm e}$ to $\mathcal{H}$ equipped with the operator norm.

Remark 2.11. The bound (2.31) displays an interesting phenomenon. Adiabatic decoupling relies on a separation of time-scales. In the present setting this separation comes from the fact that the nuclei move slowly compared to the electrons. However, this is only true if the kinetic energies of nuclei and electrons are of the same order of magnitude. But the quadratic dispersion allows the nuclei to become arbitrarily fast and as a consequence, the separation of time scales breaks down and with it adiabatic decoupling. Hence (2.31) holds only uniformly for bounded kinetic energies of the nuclei as expressed by the $\mathcal{L}(H^{2,\varepsilon} \otimes \mathcal{H}_\mathrm{e}, \mathcal{H})$ norm: Bounding $\|\psi_0\|_{H^{2,\varepsilon}}$ for the initial wave function ψ_0 by a constant independent of ε corresponds to bounding the initial velocities of the nuclei on the *macroscopic* time-scale by a constant independent of ε, since

$$\begin{aligned} \varepsilon^2\, p^2 \sim \text{const.} \quad &\Rightarrow \quad p \sim \frac{1}{\varepsilon} \quad \Rightarrow \quad v_\mathrm{micro} = \frac{p}{m_\mathrm{n}} \sim \varepsilon \\ &\Rightarrow \quad v_\mathrm{macro} = \frac{v_\mathrm{micro}}{\varepsilon} \sim \text{const.} \end{aligned}$$

The additional factor $|t|^2$ in the growth of the error in time reflects the possibility that the momenta of the nuclei grow proportional to $|t|$ as they are subject to bounded forces.

In Chapter 5 we discuss the massless Nelson model, which bears some similarities to the Born-Oppenheimer setting. There however, the corresponding dispersion of the slow degrees of freedom grows only linearly and their velocities are thus uniformly bounded. As a consequence, adiabatic decoupling holds uniformly for all initial states in this case.

Of course, a bound on the *total* energy of the system, nuclei plus electrons, as in (2.32) implies a uniform bound also on the kinetic energy of the nuclei and thus adiabatic decoupling holds uniformly again on the finite energy subspaces. ♢

Proof. It follows as in the proof of Theorem 2.2 that $P_*(\cdot) \in C^3_\mathrm{b}(\mathbb{R}^d, \mathcal{L}(\mathcal{H}_\mathrm{e}))$, since $H_\mathrm{e}(\cdot) \in C^3_\mathrm{b}(\mathbb{R}^d, \mathcal{L}(\mathcal{D}, \mathcal{H}_\mathrm{e}))$.

We first show that $H^\varepsilon_\mathrm{diag}$ is self-adjoint on the domain of H^ε. One has

$$\begin{aligned} H^\varepsilon - H^\varepsilon_\mathrm{diag} &= P_*^\perp\, H^\varepsilon\, P_* + \text{ adj.} \\ &= P_*^\perp \left[\frac{\varepsilon^2}{2} \Big(-\mathrm{i}\nabla_x + A(x) \Big)^2, P_* \right] P_* + \text{ adj.} \end{aligned} \tag{2.33}$$

Let $D_A = -\mathrm{i}\nabla_x + A(x)$. Then the commutator is easily calculated as

$$\left[\frac{\varepsilon^2}{2} (D_A \otimes \mathbf{1})^2, P_* \right] = -\mathrm{i}\,\varepsilon\, (\nabla_x P_*) \cdot (\varepsilon D_A \otimes \mathbf{1}) + \mathcal{O}(\varepsilon^2) \tag{2.34}$$

$$= -\varepsilon\, (\nabla_x P_*) \cdot (\varepsilon \nabla_x \otimes \mathbf{1}) + \mathcal{O}(\varepsilon^2)\,, \tag{2.35}$$

where $\mathcal{O}(\varepsilon^2)$ holds in the norm of $\mathcal{L}(\mathcal{H})$ as $\varepsilon \to 0$. For (2.34) and (2.35) it was used that $A(x)$ and $P_*(x)$ are both differentiable with bounded derivatives

and that $A(x)$ commutes with P_*. To see that $H^\varepsilon_{\rm diag}$ is self-adjoint on $D(H^\varepsilon)$, note that $-\mathrm{i}\varepsilon\nabla_x$ is bounded with respect to $\varepsilon^2\Delta_x$ with relative bound 0 and thus that for $\psi \in D(H^\varepsilon)$

$$\begin{aligned}\|(\varepsilon^2\Delta_x \otimes \mathbf{1})\,\psi\| &\leq c_1\,\left(\|(\varepsilon^2 D_A^2 \otimes \mathbf{1})\,\psi\| + \|\psi\|\right)\\ &\leq c_2\,\left(\|(\varepsilon^2 D_A^2 \otimes \mathbf{1} + \mathbf{1}\otimes H_{\rm e0})\,\psi\| + \|\psi\|\right)\\ &\leq c_3\,\left(\|H^\varepsilon\,\psi\| + \|\psi\|\right),\end{aligned} \tag{2.36}$$

where we used that also $H_{\rm e0}$ is bounded from below and that $H_{\rm e1}$ is bounded. Hence $H^\varepsilon - H^\varepsilon_{\rm diag}$ is infinitesimally operator bounded with respect to H^ε, consequently $H^\varepsilon_{\rm diag}$ is self-adjoint on $D(H^\varepsilon)$.

By the standard argument we find for (2.31) on $D(H^\varepsilon)$ that

$$\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm diag}t/\varepsilon} - \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} = \frac{\mathrm{i}}{\varepsilon}\,\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm diag}t/\varepsilon}\int_0^t \mathrm{d}t'\,\mathrm{e}^{\mathrm{i}H^\varepsilon_{\rm diag}t'/\varepsilon}\left(H^\varepsilon - H^\varepsilon_{\rm diag}\right)\mathrm{e}^{-\mathrm{i}H^\varepsilon t'/\varepsilon}. \tag{2.37}$$

Equations (2.33) and (2.35) in (2.37) give

$$\begin{aligned}&P_*^\perp\left(\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm diag}t/\varepsilon} - \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}\right) =\\ &= -\mathrm{i}\,\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm diag}t/\varepsilon}\int_0^t \mathrm{d}t'\,\mathrm{e}^{\mathrm{i}H^\varepsilon_{\rm diag}t'/\varepsilon}\,P_*^\perp\,(\nabla_x P_*)\,P_*\,\cdot\,(\varepsilon\nabla_x\otimes\mathbf{1})\,\mathrm{e}^{-\mathrm{i}H^\varepsilon t'/\varepsilon}\\ &\quad + \mathcal{O}(\varepsilon|t|),\end{aligned} \tag{2.38}$$

where we used that the term of order $\mathcal{O}(\varepsilon^2)$ in (2.35) yields a term of order $O(\varepsilon|t|)$ after integration, since all other expressions in the integrand are bounded uniformly in time. In (2.38) and in the following we omit the adjoint term from (2.33) and thus consider the difference of the groups projected to $P_*^\perp\mathcal{H}$ only. The argument for the difference projected on $P_*\mathcal{H}$ goes through analogously by taking adjoints at the appropriate places.

Compared to (2.22), the situation is slightly more involved this time, since the integrand is $\mathcal{O}(\varepsilon)$ not as a bounded operator, but only in the norm of $\mathcal{L}(H^{1,\varepsilon}\otimes\mathcal{H}_{\rm e},\mathcal{H})$. However, we can still define

$$F(x) = \frac{1}{2\pi\mathrm{i}}\oint_{\Gamma(x)}\mathrm{d}\zeta\,P_*^\perp(x)\,R(\zeta,x)\,(\nabla R)(\zeta,x)$$

as in (2.23), where we recall that $R(\zeta,x) = (H_{\rm e}(x)-\zeta)^{-1}$. As in (2.11) one concludes that

$$[\,H_{\rm e}(x),\,F(x)\,] = P_*^\perp(x)\,(\nabla P_*)(x)\,P_*(x). \tag{2.39}$$

By assumption we have that $H_{\rm e}(\cdot)\in C^3_{\rm b}(\mathbb{R}^d,\mathcal{L}(\mathcal{D},\mathcal{H}_{\rm e}))$, which implies $F(x)\in C^2_{\rm b}(\mathbb{R}^d,\mathcal{L}(\mathcal{H}_{\rm e})^{\oplus d})$, cf. Lemma 2.4. As a consequence we obtain that the commutator

$$\left[\frac{\varepsilon^2}{2}\,D_A^2\otimes\mathbf{1},\,F\right]=-\varepsilon\,(\nabla_x F)\,\cdot\,(\varepsilon\nabla_x\otimes\mathbf{1})+\mathcal{O}(\varepsilon^2)\tag{2.40}$$

is $\mathcal{O}(\varepsilon)$ in the norm of $\mathcal{L}(H^{1,\varepsilon}\otimes\mathcal{H}_{\mathrm{e}},\mathcal{H})$. Combining (2.39) and (2.40) one finds that

$$[\,H^\varepsilon,\,F\,]=P_*^\perp\,(\nabla_x P_*)\,P_*+\mathcal{O}(\varepsilon)$$

with $\mathcal{O}(\varepsilon)$ in the norm of $\mathcal{L}(H^{1,\varepsilon}\otimes\mathcal{H}_{\mathrm{e}},\mathcal{H})$. Since $\nabla_x H_{\mathrm{e}}\in\mathcal{L}(\mathcal{H})$, a short calculation shows that $[H^\varepsilon,\varepsilon\nabla_x\otimes\mathbf{1}]=\mathcal{O}(\varepsilon)$ in $\mathcal{L}(H^{1,\varepsilon}\otimes\mathcal{H}_{\mathrm{e}},\mathcal{H})$. Hence we obtain for

$$G=F\cdot(\varepsilon\nabla_x\otimes\mathbf{1})$$

that

$$\begin{aligned}[\,H^\varepsilon,\,G\,]&=[\,H^\varepsilon,\,F\,]\cdot(\varepsilon\nabla_x\otimes\mathbf{1})+F\cdot[\,H^\varepsilon,\,\varepsilon\nabla_x\otimes\mathbf{1}\,]\\&=\,P_*^\perp\,(\nabla_x P_*)\,P_*\,\cdot\,(\varepsilon\nabla_x\otimes\mathbf{1})+\mathcal{O}(\varepsilon)\end{aligned}$$

with $\mathcal{O}(\varepsilon)$ in the norm of $\mathcal{L}(H^{2,\varepsilon}\otimes\mathcal{H}_{\mathrm{e}},\mathcal{H})$. Let

$$A(t)=-\mathrm{i}\,\varepsilon\,\mathrm{e}^{\mathrm{i}H^\varepsilon t/\varepsilon}\,G\,\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}\,,$$

such that on a suitable dense domain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}A(t)&=\mathrm{e}^{\mathrm{i}H^\varepsilon t/\varepsilon}\,[\,H^\varepsilon,\,G\,]\,\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}\qquad(2.41)\\&=\mathrm{e}^{\mathrm{i}H^\varepsilon t/\varepsilon}\,P_*^\perp\,(\nabla_x P_*)\,P_*\,\cdot\,(\varepsilon\nabla_x\otimes\mathbf{1})\,\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}+\mathcal{O}\big(\varepsilon(1+|t|)^2\big)\,,\end{aligned}$$

where $\mathcal{O}(\varepsilon(1+|t|)^2)$ holds in the norm of $\mathcal{L}(H^{2,\varepsilon}\otimes\mathcal{H}_{\mathrm{e}},\mathcal{H})$. The additional factor of $(1+|t|)^2$ comes from the fact that

$$\left\|\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}\right\|_{\mathcal{L}(H^{2,\varepsilon}\otimes\mathcal{H}_{\mathrm{e}})}\le\,c\,(1+|t|)^2\tag{2.42}$$

for some constant $c<\infty$, i.e. the kinetic energy of the nuclei may grow in time. Using $\|A\|_\infty=C<\infty$ and

$$\|\,[\,(\varepsilon D_A\otimes\mathbf{1}),\,H^\varepsilon\,]\,\|_{\mathcal{L}(\mathcal{H})}\,\le\,\widetilde{C}\,\varepsilon\,,$$

the analogous bound to (2.42) in $\mathcal{L}(H^{1,\varepsilon}\otimes\mathcal{H}_{\mathrm{e}},\mathcal{H})$ follows from

$$\begin{aligned}\left\|(\varepsilon\nabla_x\otimes\mathbf{1})\,\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}\,\psi\right\|&\le\left\|(\varepsilon D_A\otimes\mathbf{1})\,\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}\,\psi\right\|+\left\|(\varepsilon A\otimes\mathbf{1})\,\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}\,\psi\right\|\\&\le\,\|(\varepsilon D_A\otimes\mathbf{1})\,\psi\|+\left\|\Big[(\varepsilon D_A\otimes\mathbf{1}),\,\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}\Big]\,\psi\right\|+C\,\|\psi\|\\&\le\,\|(\varepsilon\nabla_x\otimes\mathbf{1})\,\psi\|\,+\,\widetilde{C}\,|t|\,\|\psi\|\,+\,2\,C\,\|\psi\|\end{aligned}$$

for $\psi\in H^1\otimes\mathcal{H}_{\mathrm{e}}$. A repetition of the same argument yields (2.42).

For the following we use the abbreviations $\widetilde{\mathcal{L}}_1=\mathcal{L}(H^{1,\varepsilon}\otimes\mathcal{H}_{\mathrm{e}},\mathcal{H})$ and $\widetilde{\mathcal{L}}_2=\mathcal{L}(H^{2,\varepsilon}\otimes\mathcal{H}_{\mathrm{e}},\mathcal{H})$. Notice the natural bounded inclusions $\mathcal{L}\subset\widetilde{\mathcal{L}}_1\subset\widetilde{\mathcal{L}}_2$. With this in mind we continue (2.38) and find

$$\left\| P_*^\perp \left(\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{diag}} t/\varepsilon} - \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} \right) \right\|_{\tilde{\mathcal{L}}_2} = \tag{2.43}$$
$$= \left\| \int_0^t \mathrm{d}t' \, \mathrm{e}^{\mathrm{i}H^\varepsilon_{\mathrm{diag}} t'/\varepsilon} \, \mathrm{e}^{-\mathrm{i}H^\varepsilon t'/\varepsilon} \left(\frac{\mathrm{d}}{\mathrm{d}t'} A(t') \right) \right\|_{\tilde{\mathcal{L}}_2} + \mathcal{O}\big(\varepsilon|t|(1+|t|)^2\big) \, .$$

Again integration by parts yields

$$\left\| P_*^\perp \left(\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{diag}} t/\varepsilon} - \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} \right) \right\|_{\tilde{\mathcal{L}}_2} = \tag{2.44}$$
$$= \varepsilon \left\| G \, \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} \right\|_{\tilde{\mathcal{L}}_2} + \varepsilon \left\| \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{diag}} t/\varepsilon} \, G \right\|_{\tilde{\mathcal{L}}_2}$$
$$+ \left\| \int_0^t \mathrm{d}t' \, \mathrm{e}^{\mathrm{i}H^\varepsilon_{\mathrm{diag}} t'/\varepsilon} \big(H^\varepsilon - H^\varepsilon_{\mathrm{diag}} \big) G \, \mathrm{e}^{-\mathrm{i}H^\varepsilon t'/\varepsilon} \right\|_{\tilde{\mathcal{L}}_2} + \mathcal{O}\big(\varepsilon|t|(1+|t|)^2\big) \, . \tag{2.45}$$

From the estimate below (2.42) and $G \in \mathcal{L}_1$ we conclude that

$$\varepsilon \left\| G \, \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} \right\|_{\tilde{\mathcal{L}}_2} + \varepsilon \left\| \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{diag}} t/\varepsilon} \, G \right\|_{\tilde{\mathcal{L}}_2} \leq \varepsilon \left\| G \, \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} \right\|_{\tilde{\mathcal{L}}_1} + \varepsilon \, \| G \|_{\tilde{\mathcal{L}}_1}$$
$$= \mathcal{O}\big(\varepsilon(1+|t|)\big) \, .$$

For the remaining term in (2.44) note that $G \in \mathcal{L}(H^{2,\varepsilon} \otimes \mathcal{H}_{\mathrm{e}}, H^{1,\varepsilon} \otimes \mathcal{H}_{\mathrm{e}})$ and that $\| H^\varepsilon - H^\varepsilon_{\mathrm{diag}} \|_{\tilde{\mathcal{L}}_1} = \mathcal{O}(\varepsilon)$, as we saw in (2.33) and (2.35). Again with (2.42) we obtain that

$$\left\| P_*^\perp \left(\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{diag}} t/\varepsilon} - \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} \right) \right\|_{\tilde{\mathcal{L}}_2} \leq C \, \varepsilon \, (1+|t|)^3 \, ,$$

which gives one half of (2.31). The estimate for the second part follows analogously.

Finally, (2.32) is a corollary of the previous proof, where one uses that $\mathcal{E}(H^\varepsilon)$ commutes with $\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}$ and that, according to (2.36),

$$\|(\varepsilon^2 \Delta_x \otimes \mathbf{1}) \, \mathcal{E}(H^\varepsilon) \, \psi\| \leq c_3 \, \big(\|H^\varepsilon \, \mathcal{E}(H^\varepsilon) \, \psi\| + \|\psi\| \big) \leq c_4 \, (|\mathcal{E}| + 1) \, \|\psi\| \, .$$

□

2.3.2 Local results and effective dynamics

In general the eigenvalues of the electronic Hamiltonian $H_{\mathrm{e}}(x)$ form isolated energy bands only locally in nucleonic configuration space $\mathbb{R}^d$. This is because eigenvalues cross or merge into the continuous spectrum, cf. Figure 2.2. For the following we thus only assume that the gap condition is satisfied locally for some open region $\Lambda \subset \mathbb{R}^d$ and we consider solutions of the Schrödinger equation which are initially and stay supported in Λ, at least approximately, for some time.

In order to control the maximal time for which a given initial wave function supported in Λ stays supported in Λ, we apply techniques from semiclassical analysis. To this end we have to approximate the diagonal Hamiltonian by an effective Hamiltonian to which semiclassical analysis can be applied. We shall see that this is possible whenever $\sigma_*(x) = \{E(x)\}$ is an eigenvalue for all $x \in \Lambda$.

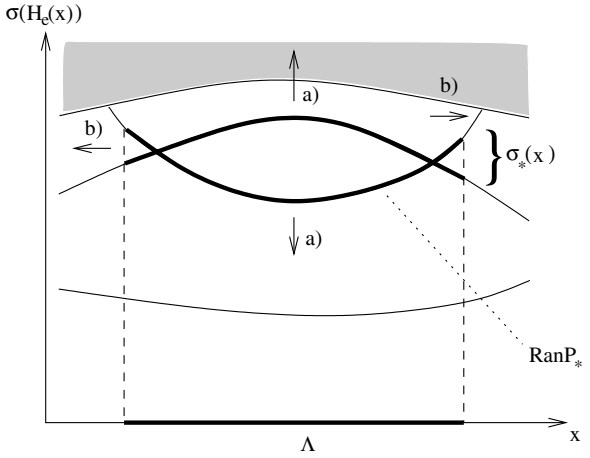

Fig. 2.2. The wave function can leave RanP_* in two different ways. Either by transitions to other bands (a) or through the boundary of Λ (b).

For the following Λ may thus be any open subset of $\mathbb{R}^d$ and for such a Λ we assume $\mathbf{H}_\infty$ and **Gap** with $\sigma_*(x) = \{E(x)\}$ an eigenvalue of finite and necessarily constant multiplicity ℓ. We also assume that Λ is connected. Otherwise one could treat each connected component separately. In order to simplify the presentation at this point and not to introduce too many new complications at one time we also restrict ourselves to the case $\ell = 1$. In view of the results in Section 3.4 the generalization of the following to the case of any $\ell \in \mathbb{N}$ is straightforward. The effective Hamiltonian in the general case can be found in Section 4.2.

By the general argument given in the proof of Theorem 2.2, $\mathbf{H}_\infty$ and **Gap** on Λ imply that the corresponding family of projections satisfies $P_*(\cdot) \in C^\infty_{\mathrm{b}}(\Lambda, \mathcal{L}(\mathcal{H}_{\mathrm{e}}))$. As explained in Section 1.2., the key idea for constructing an effective dynamics on the decoupled subspace $P_*\mathcal{H}$ is to unitarily map it to the reference subspace $L^2(\Lambda)^{\oplus\ell}$, i.e. $L^2(\Lambda)$ for the moment. To this end we need a smooth version $\chi(\cdot) \in C^\infty_{\mathrm{b}}(\Lambda, \mathcal{H}_{\mathrm{e}})$ of the eigenvectors $\chi(x)$ corresponding to $E(x)$. Such a smooth family of eigenvectors can be regarded as a smooth section of the complex line bundle over Λ defined by P_* and it exists whenever the latter is globally trivial. A sufficient condition for the bundle to be trivial

is that the base space Λ is contractible. As to be discussed below, there are some relevant examples where Λ is not contractible, but the bundle is still trivial. For a more detailed discussion of the bundle theoretic argument see Remark 3.17 in Chapter 3.

Given a smooth and normalized family of eigenvectors $\chi(x)$ one has $\mathrm{Re}\langle\chi(x), \nabla_x\chi(x)\rangle = 0$, but, in general, $\mathrm{Im}\langle\chi(x), \nabla_x\chi(x)\rangle \neq 0$. In the following we distinguish two cases: Either it is possible to achieve

$$\mathrm{Im}\langle\widetilde{\chi}(x), \nabla_x\widetilde{\chi}(x)\rangle = 0$$

by a smooth gauge transformation $\chi(x) \to \widetilde{\chi}(x) = \mathrm{e}^{\mathrm{i}\theta(x)}\chi(x)$ or not. In the latter case

$$\mathcal{A}(x) := \mathrm{i}\langle\chi(x), \nabla_x\chi(x)\rangle$$

is the gauge potential of a connection on the trivial complex line bundle over Λ, the Berry connection, and has to be taken into account in the definition of the effective operator

$$H^{\varepsilon}_{\mathrm{BO}} := \frac{\varepsilon^2}{2}\Big(-i\nabla_x + A(x) - \mathcal{A}(x)\Big)^2 + E(x) \tag{2.46}$$

with domain $H^2(\mathbb{R}^d)$. Thus $\mathcal{A}$ acts similar to an external magnetic vector potential. However, while A comes from a connection of a line bundle over $\mathbb{R}^3$, $\mathcal{A}$ comes from a connection of a line bundle over $\mathbb{R}^d$. Although A and $\mathcal{A}$ appear in $H^{\varepsilon}_{\mathrm{BO}}$ with an ε in front only, and therefore are not retained in the semiclassical limit to leading order, they do contribute to the solution of the Schrödinger equation for times of order ε^{-1}. If the full Hamiltonian is real in position representation, as it is the case for the Hamiltonians considered in the introduction whenever $A = 0$, then $\chi(x)$ can be chosen real-valued. If, in addition, Λ is contractible, the existence of a smooth version of $\chi(x)$ with $\mathrm{Im}\langle\chi(x), \nabla_x\chi(x)\rangle = 0$ follows. In Section 2.3.4 we give an example showing the importance of the geometric potential in the Born-Oppenheimer Hamiltonian (2.46).

To define $H^{\varepsilon}_{\mathrm{BO}}$ on $L^2(\mathbb{R}^d)$ through (2.46), the functions $E(x)$ and $\mathcal{A}(x)$, which are a priori defined on Λ only, must be continued to functions on $\mathbb{R}^d$. Hence we arbitrarily extend $E(x)$ and $\mathcal{A}(x)$ to functions in $C^{\infty}_{\mathrm{b}}(\mathbb{R}^d)$ by modifying them, if necessary, on $\Lambda \setminus (\Lambda - \delta/5)$ (cf. (2.50)) for some $\delta > 0$. The parameter δ will be fixed in the formulation of Theorem 2.14 and will appear in several places. It controls how close the states are allowed to come to $\partial\Lambda$.

The generic example for the Berry phase is a band crossings of codimension 2 (cf. [ShWi, Ha$_3$, FeGe, FeLa, LaTe]). If $E(x)$ is an isolated energy band except for a codimension 2 crossing, then $\Lambda = \mathbb{R}^d \setminus \{\text{closed neighborhood of the crossing}\}$ is no longer contractible, but the line bundle is still trivial. Although the underlying Hamiltonian is real, the Berry connection cannot be gauged away. Within the time-independent Born-Oppenheimer approximation Herrin and Howland [HeHo] study a model with a nontrivial eigenvector bundle.

With the fixed choice for $\chi(x)$ we have

$$P_*\mathcal{H} = \left\{ \int_\Lambda^\oplus \mathrm{d}x\, \phi(x)\chi(x) : \phi \in L^2(\Lambda) \right\} \subset \mathcal{H}\,. \tag{2.47}$$

Thus there is a natural identification $\mathcal{U} : P_*\mathcal{H} \to L^2(\mathbb{R}^d)$ connecting the relevant subspace on which the full quantum evolution takes place and the Hilbert space $L^2(\mathbb{R}^d)$ on which the effective Born-Oppenheimer evolution is defined. According to (2.47), we set

$$\mathcal{U}(\phi\chi) = \phi\,, \qquad \text{i.e.} \quad (\mathcal{U}P_*\,\psi\,)(x) = \langle\, \chi(x)\,,\, (P_*\,\psi)(x)\,\rangle_{\mathcal{H}_\mathrm{e}}\,.$$

Its adjoint $\mathcal{U}^* : L^2(\mathbb{R}^d) \to P_*\mathcal{H}$ is given by

$$\mathcal{U}^*\phi = \int_\Lambda^\oplus \mathrm{d}x\, \phi(x)\chi(x)\,.$$

Clearly $\mathcal{U}$ is an isometry and $\mathcal{U}^*\mathcal{U} = \mathbf{1}$ on $P_*\mathcal{H}$. But $\mathcal{U}$ is not surjective and thus not unitary.

By construction, $\mathrm{e}^{-\mathrm{i}H^\varepsilon_\mathrm{BO}t/\varepsilon}$ can be expected to be a good approximation to the true dynamics only as long as the wave function of the nuclei is supported in Λ modulo errors of order ε. Since $H^\varepsilon_\mathrm{BO}$ is a standard semiclassical operator, the x-support of solutions of the effective Schrödinger equation

$$\mathrm{i}\,\varepsilon\,\frac{\mathrm{d}}{\mathrm{d}t}\,\phi(t) = H^\varepsilon_\mathrm{BO}\,\phi(t)\,, \quad \phi(0) \in L^2(\mathbb{R}^d) \tag{2.48}$$

can be calculated approximately from the classical dynamics generated by the principal symbol $H_\mathrm{cl}(q,p) = \frac{1}{2}p^2 + E(q)$ of $H^\varepsilon_\mathrm{BO}$ on phase space $Z := \mathbb{R}^d \times \mathbb{R}^d$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\,q = p\,, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\,p = -\nabla E(q)\,. \tag{2.49}$$

The solution flow to (2.49) exists for all times and will be denoted by Φ^t.

In order to make these notions more precise, we need to introduce some notation. For details we refer to Appendix A. However, for the following only a few basic results are needed, which we repeat here for the convenience of the reader.

For the convenience of the reader we recall here that the Weyl quantization $\widehat{a}$ of a function (= symbol) $a \in C^\infty_\mathrm{b}(Z)$ is the linear operator

$$(\widehat{a}\phi)\,(x) = (2\pi)^{-d} \int_{\mathbb{R}^d} \mathrm{d}y\,\mathrm{d}k\, a\left(\frac{x+y}{2}, \varepsilon\, k\right) \mathrm{e}^{-\mathrm{i}(x-y)\cdot k}\phi(y)\,,$$

as acting on Schwartz functions. $\widehat{a}$ extends to $\mathcal{L}(L^2(\mathbb{R}^d))$ with operator norm bounded uniformly in ε.

Using Weyl quantization, one can define approximate projections on sets of wave functions with "phase space support" in a compact set $\Gamma \subset Z$. To this end let for $\Gamma \subset \mathbb{R}^m$, $m \in \mathbb{N}$, and for $\alpha > 0$

$$\Gamma - \alpha := \left\{ z \in \Gamma : \inf_{w \in \mathbb{R}^m \setminus \Gamma} |w - z| \geq \alpha \right\} . \tag{2.50}$$

Definition 2.12. *An* approximate characteristic function $\mathbf{1}_{(\Gamma,\alpha)} \in C_{\mathrm{b}}^{\infty}(\mathbb{R}^m)$ *of a set* $\Gamma \subset \mathbb{R}^m$ *with margin* α *is defined by the requirement that* $\mathbf{1}_{(\Gamma,\alpha)}|_{\Gamma-\alpha} = 1$ *and* $\mathbf{1}_{(\Gamma,\alpha)}|_{\mathbb{R}^m \setminus \Gamma} = 0$.

If $\mathbf{1}_{(\Gamma,\alpha)}$ *is an approximate characteristic function, then the corresponding* approximate projection *is defined as its Weyl quantization* $\widehat{\mathbf{1}_{(\Gamma,\alpha)}}$. *We will say that functions in* $\widehat{\mathbf{1}_{(\Gamma,\alpha)}} L^2(\mathbb{R}^m)$ *have phase space support in* Γ. ♢

For $\Gamma \subset Z$ we will use the abbreviations

$$\Gamma_q := \left\{ q \in \mathbb{R}^d : \, (q,p) \in \Gamma \text{ for some } p \in \mathbb{R}^d \right\} ,$$
$$\Gamma_p := \left\{ p \in \mathbb{R}^d : \, (q,p) \in \Gamma \text{ for some } q \in \mathbb{R}^d \right\} .$$

Let the phase space support Γ of the initial wave function be such that $\Gamma_q \subset \Lambda - \delta$. Then the maximal time interval for which the x-support of the wave function of the nuclei stays in Λ up to errors of order ε can be written as

$$I_{\max}^{\delta}(\Gamma, \Lambda) := [T_-^{\delta}(\Gamma, \Lambda), T_+^{\delta}(\Gamma, \Lambda)] ,$$

where the "first hitting times" $T_{\pm}$ are defined by the classical dynamics through

$$T_+^{\delta}(\Gamma, \Lambda) := \sup \left\{ t \geq 0 : \, \left(\Phi^{t'}(\Gamma) \right)_q \subseteq \Lambda - \delta \ \forall\, t' \in [0,t] \right\}$$

and $T_-^{\delta}(\Gamma, \Lambda)$ analogously for negative times. These are just the first times for a particle starting in Γ to hit the boundary of $\Lambda - \delta$ when dragged along the classical flow Φ^t.

The following proposition, which is an immediate consequence of Egorov's Theorem, cf. Section 3.4 or e.g. [Ro], shows that for times in $I_{\max}^{\delta}(\Gamma, \Lambda)$ the support of the wave function of the nuclei stays indeed in $\Lambda - \delta$, up to errors of order ε uniformly on $\widehat{\mathbf{1}_{(\Gamma,\alpha)}}$ for any approximate projection $\widehat{\mathbf{1}_{(\Gamma,\alpha)}}$.

Proposition 2.13. *Let* $\Gamma \subset Z$ *be such that* $\Gamma_q \subset \Lambda - \delta$ *and let* $\mathbf{1}_{\Lambda-\delta}$ *denote multiplication with the characteristic function of* $\Lambda - \delta$ *on* $L^2(\mathbb{R}^d)$. *For any approximate projection* $\widehat{\mathbf{1}_{(\Gamma,\alpha)}}$ *and any bounded interval* $I \subseteq I_{\max}^{\delta}(\Gamma, \Lambda)$ *there is a constant* $C < \infty$ *such that for all* $t \in I$

$$\left\| \left(\mathbf{1} - \mathbf{1}_{\Lambda-\delta} \right) \mathrm{e}^{-\mathrm{i} H_{\mathrm{BO}}^{\varepsilon} t/\varepsilon} \, \widehat{\mathbf{1}_{(\Gamma,\alpha)}} \right\|_{\mathcal{L}(L^2(\mathbb{R}^d))} \leq C \, \varepsilon .$$

An approximate projection on Γ in $\mathcal{H}$ is defined as

$$P_{\Gamma}^{\alpha} := \mathcal{U}^* \, \mathbf{1}_{(\Lambda,\delta)} \, \widehat{\mathbf{1}_{(\Gamma,\alpha)}} \, \mathcal{U} \, P_* ,$$

where $\widehat{\mathbf{1}_{(\Gamma,\alpha)}}$ is an approximate projection on Γ according to Definition 2.12 and $\mathbf{1}_{(\Lambda,\delta)}$ is an approximate characteristic function for Λ. Using the latter instead of the sharp cutoff from $\mathcal{U}^*$ makes $P_{\Gamma}^{\alpha}\mathcal{H}$ a bounded set in $H^{2,\varepsilon} \otimes \mathcal{H}_{\mathrm{e}}$ whenever Γ_p is a bounded set.

Theorem 2.14. *Assume* $\mathbf{H}_\infty$ *and* **Gap on** Λ *with* $dim(P_*(x)\mathcal{H}) = 1$ *for some open* $\Lambda \subseteq \mathbb{R}^d$. *Let* $\Gamma \subset Z$ *be such that* $\Gamma_q \subset \Lambda - \delta$ *for some* $\delta > 0$ *and* Γ_p *bounded. For any approximate projection* P_Γ^α *and any bounded interval* $I \subseteq I_{\max}^\delta(\Gamma, \Lambda)$ *there is a constant* $C < \infty$ *such that for all* $t \in I$

$$\left\| \left(\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} - \mathcal{U}^* \, \mathrm{e}^{-\mathrm{i}H_{\mathrm{BO}}^\varepsilon t/\varepsilon} \, \mathcal{U} \right) P_\Gamma^\alpha \right\|_{\mathcal{L}(\mathcal{H})} \leq C\varepsilon \,. \tag{2.51}$$

Theorem 2.14 establishes that the electrons adiabatically follow the motion of the nuclei up to errors of order ε as long as the leaking through the boundary of Λ is small. The semiclassics was used only to control such a leaking uniformly. However, for $H_{\mathrm{BO}}^\varepsilon$ the limit $\varepsilon \to 0$ is a semiclassical limit and beyond the mere support of the wave function more detailed information is available.

Proof. To prove Theorem 2.14 we proceed along the same lines as in the global case, with the one modification that we use Proposition 2.13 to control the flux out of $\partial\Lambda$. However, one cannot use $P_* = \int_\Lambda^\oplus \mathrm{d}x \, P_*(x)$ to define $H_{\mathrm{diag}}^\varepsilon$ anymore, because the functions in its range would not be in the range of H^ε and some smoothing in the cutoff is needed. For $i \in \{0, 1, 2, 3\}$ let $\mathbf{1}_i = \mathbf{1}_{(\Lambda - \frac{4-i}{5}\delta, \frac{1}{5}\delta)}$ be approximate characteristic functions according to Definition 2.12. Then the smoothed projections are defined with $P_i(x) = \mathbf{1}_i(x) \, P_*(x)$ as $P_i = \int^\oplus \mathrm{d}x \, P_i(x)$. In the following it will be used that for $i < j$ we have $P_i P_j = P_j P_i = P_i$ and hence $(1 - P_j)P_i = P_i(1 - P_j) = 0$.

As the first step Proposition 2.13 yields

$$\begin{aligned} &\left(\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} - \mathcal{U}^* \, \mathrm{e}^{-\mathrm{i}H_{\mathrm{BO}}^\varepsilon t/\varepsilon} \, \mathcal{U} \right) P_\Gamma^\alpha \\ &\qquad = \left(\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} - P_1 \, \mathcal{U}^* \, \mathrm{e}^{-\mathrm{i}H_{\mathrm{BO}}^\varepsilon t/\varepsilon} \, \mathcal{U} \right) P_\Gamma^\alpha + \mathcal{O}(\varepsilon) \,. \end{aligned} \tag{2.52}$$

We will also use the fact that the phase space support of the initial wave function lies in Γ and has thus bounded energy with respect to H_{cl}. Let $E := \sup_{z \in \Gamma} H_{\mathrm{cl}}(z) < \infty$, let $\mathbf{1}_{((-\infty, E+\alpha), \alpha)}$ be a smooth characteristic function on $\mathbb{R}$ and let $\mathcal{E} = \mathcal{W}\Big(\mathbf{1}_{((-\infty, E+\alpha), \alpha)}(H_{\mathrm{cl}}(\cdot)) \Big)$, where $\mathcal{W}$ denotes Weyl quantization. Then standard results from semiclassical analysis imply the following relations.

Proposition 2.15. *The following equalities hold in the norm of* $\mathcal{L}(L^2(\mathbb{R}^d))$*:*

(i) $\widehat{\mathbf{1}_{(\Gamma,\alpha)}} = \mathcal{E} \, \widehat{\mathbf{1}_{(\Gamma,\alpha)}} + \mathcal{O}(\varepsilon)$*;*
(ii) $\mathrm{e}^{-\mathrm{i}H_{\mathrm{BO}}^\varepsilon t/\varepsilon} \, \mathcal{E} = \mathcal{E} \, \mathrm{e}^{-\mathrm{i}H_{\mathrm{BO}}^\varepsilon t/\varepsilon} + \mathcal{O}(\varepsilon)$ *uniformly for* $t \in I$*;*
(iii) $[\, H_{\mathrm{BO}}^\varepsilon, \, \mathcal{E} \,] = \mathcal{O}(\varepsilon^2)$*;*
(iv) $\mathcal{E} \in \mathcal{L}(L^2(\mathbb{R}^d), H^{2,\varepsilon})$.

Proposition (2.15) (i), (iii) and (iv) are direct consequences of the product rule for pseudo-differential operators, see Proposition A.15, and (ii) is again Egorov's Theorem.

With the help of Proposition 2.15 (i) and (ii) we can continue (2.52) and obtain

$$\begin{aligned}\Big(\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} - P_1\,\mathcal{U}^*\,\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{BO}}t/\varepsilon}\,\mathcal{U}\Big)\;P_\Gamma^\alpha \\ = \Big(\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} - P_1\,\mathcal{U}^*\,\mathcal{E}\,\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{BO}}t/\varepsilon}\,\mathcal{U}\Big)\;P_\Gamma^\alpha + \mathcal{O}(\varepsilon)\,.\end{aligned}$$

From this we proceed as in the globally isolated band case and write

$$\begin{aligned}&\Big(\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} - P_1\,\mathcal{U}^*\,\mathcal{E}\,\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{BO}}t/\varepsilon}\,\mathcal{U}\Big)\;P_\Gamma^\alpha \\ &= -\mathrm{i}\,\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}\int_0^t \mathrm{d}t'\,\mathrm{e}^{\mathrm{i}H^\varepsilon t'/\varepsilon}\,\big(H^\varepsilon\,P_1\,\mathcal{U}^*\,\mathcal{E}\;-\;P_1\,\mathcal{U}^*\,\mathcal{E}\,H^\varepsilon_{\mathrm{BO}}\big)\,\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{BO}}t'/\varepsilon}\,\mathcal{U}\,P_\Gamma^\alpha \\ &= -\mathrm{i}\,\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}\int_0^t \mathrm{d}t'\,\mathrm{e}^{\mathrm{i}H^\varepsilon t'/\varepsilon}\,\big(H^\varepsilon\;-\;H^\varepsilon_{\mathrm{diag}}\big)\,P_1\,\mathcal{U}^*\,\mathcal{E}\,\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{BO}}t'/\varepsilon}\,\mathcal{U}\,P_\Gamma^\alpha \qquad (2.53)\\ &\quad -\mathrm{i}\,\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}\int_0^t \mathrm{d}t'\,\mathrm{e}^{\mathrm{i}H^\varepsilon t'/\varepsilon}\,\big(H^\varepsilon_{\mathrm{diag}}\,P_1\,\mathcal{U}^*\,\mathcal{E} - P_1\,\mathcal{U}^*\,\mathcal{E}\,H^\varepsilon_{\mathrm{BO}}\big)\,\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{BO}}t'/\varepsilon}\,\mathcal{U}\,P_\Gamma^\alpha\,, \qquad (2.54)\end{aligned}$$

where

$$H^\varepsilon_{\mathrm{diag}} := P_3\,H^\varepsilon\,P_3\,.$$

One can now show that (2.53) is bounded in norm by a constant times $\varepsilon(1+|t|)$ using exactly the same sequence of arguments as in the proof in the previous section. One must only keep track of the "hierarchy" of smoothed projections, e.g., instead of (2.33) one has

$$\big(H^\varepsilon\;-\;H^\varepsilon_{\mathrm{diag}}\big)P_1 = (1-P_3)\left[-\frac{\varepsilon^2}{2}\Delta_x\otimes\mathbf{1}, P_2\right]P_1\;+\;\mathcal{O}(\varepsilon^2).$$

The adjoint part drops out completely, because this time only the difference on the band, i.e. on $P_1\mathcal{H}$, is of interest. Note also that the smoothed projections P_i are bounded operators on the respective scaled Sobolev spaces and thus, according to Proposition 2.15 (iv), all estimates hold in the norm of $\mathcal{L}(\mathcal{H})$.

It remains to show that also (2.54) is $\mathcal{O}(\varepsilon)$. First note that, according to Proposition 2.15 (iii), commuting $\mathcal{E}$ and $H^\varepsilon_{\mathrm{BO}}$ yields an error of order $\mathcal{O}(\varepsilon^2)$ in the integrand and thus an error of order $\mathcal{O}(\varepsilon)$ after integration. For $\phi\in H^2$ we compute

$$\begin{aligned}(H^\varepsilon_{\mathrm{diag}}\,P_1\,\mathcal{U}^*\phi)(x) &= \mathbf{1}_1(x)\,E(x)\,\phi(x)\chi(x)\\ &\quad+\mathbf{1}_1(x)\left(\frac{\varepsilon^2}{2}\big(-\mathrm{i}\nabla_x+A\big)^2\,\phi\right)(x)\,\chi(x)\\ &\quad+\varepsilon\,\mathbf{1}_1(x)\,(-\mathrm{i}\varepsilon\nabla\phi)\,(x)\cdot(-\mathrm{i}\langle\chi(x),\nabla_x\chi(x)\rangle_{\mathcal{H}_{\mathrm{e}}})\;\chi(x)\\ &\quad-\mathrm{i}\,\varepsilon\,(\nabla\mathbf{1}_1)(x)\cdot(-\mathrm{i}\varepsilon\nabla\phi)\,(x)\,\chi(x)\;+\;\mathcal{O}(\varepsilon^2)\,.\end{aligned}$$

On the other hand, again for $\phi \in H^2$,

$$\begin{aligned}(P_1\,\mathcal{U}^*\,H^\varepsilon_{\rm BO}\,\phi)(x) &= \mathbf{1}_1(x)\,E(x)\,\phi(x)\chi(x)\\ &\quad+\mathbf{1}_1(x)\left(\frac{\varepsilon^2}{2}\big(-\mathrm{i}\nabla_x+A\big)^2\,\phi\right)(x)\,\chi(x)\\ &\quad-\varepsilon\,\mathbf{1}_1(x)\,(-\mathrm{i}\varepsilon\nabla\phi)\,(x)\cdot\mathcal{A}(x)\,\chi(x)\;+\;\mathcal{O}(\varepsilon^2)\,.\end{aligned}$$

Hence

$$H^\varepsilon_{\rm diag}\,P_1\,\mathcal{U}^*\mathcal{E}-P_1\,\mathcal{U}^*\,H^\varepsilon_{\rm BO}\,\mathcal{E}=-\varepsilon\,\mathcal{U}^*\,(\nabla\mathbf{1}_1)\cdot\varepsilon\nabla_x\,\mathcal{E}+\mathcal{O}(\varepsilon^2)$$

Thus the norm of (2.54) is, up to an error of order $\mathcal{O}(\varepsilon)$, bounded by the norm of

$$\mathcal{U}^*\int_0^t \mathrm{d}t'\,(\nabla\mathbf{1}_1)\cdot\varepsilon\nabla_x\,\mathcal{E}\,\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm BO}t'/\varepsilon}\,\mathcal{U}\,P^\alpha_\Gamma\,. \tag{2.55}$$

$(\nabla\mathbf{1}_1)\cdot\varepsilon\nabla_x\,\mathcal{E}$ is a bounded operator and we can apply Proposition 2.13 in the integrand of (2.55) once more, this time however with the smoothed projection P_0, and obtain

$$(2.55)\;=\;\mathcal{U}^*\int_0^t \mathrm{d}t'\,(\nabla\mathbf{1}_1)\cdot\varepsilon\nabla_x\,\mathcal{E}\,\mathbf{1}_0\,\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm BO}t'/\varepsilon}\,\mathcal{U}\,P^\alpha_\Gamma\;+\mathcal{O}(\varepsilon)=\mathcal{O}(\varepsilon). \tag{2.56}$$

The last equality in (2.56) follows from the fact that $[\varepsilon\nabla_x\,\mathcal{E},\mathbf{1}_0]=\mathcal{O}(\varepsilon)$ and that $(\nabla\mathbf{1}_1)$ and $\mathbf{1}_0$ are disjointly supported. □

2.3.3 The semiclassical limit: first remarks

The semiclassical limit of Equation (2.48) with a Hamiltonian of the form (2.46) is well understood and there is a variety of different approaches. For example one can construct approximate solutions $\phi_{q(t)}$ of (2.48) which are localized along a classical trajectory $q(t)$, i.e. along a solution of (2.49). Then it follows from Theorem 2.14 that $\phi_{q(t)}\chi$ is a solution of the full Schrödinger equation with Hamiltonian (2.27), up to an error of order ε as long as $q(t)\in\Lambda-\delta$. Roughly speaking, this coincides with the result of Hagedorn [Ha$_1$]. In applications the assumption that the wave function of the nuclei is well described by a coherent state can be too restrictive. To cope with general initial conditions one can consider the distributions of semiclassical observables, i.e. of operators obtained as Weyl quantization $\widehat{a}$ of classical phase space functions $a: Z\to\mathbb{R}$. In this short section we discuss the leading order semiclassical limit of the Schrödinger equation (2.48) based on the latter approach and show how to translate the results to the solutions of the full molecular Schrödinger equation. More details in the general case and also higher order approximations can be found in Section 3.4.

Consider a general initial wave function $\phi^\varepsilon\in L^2(\mathbb{R}^d)$, such that ϕ^ε corresponds to a probability measure $\rho_{\rm cl}(\mathrm{d}q\,\mathrm{d}p)$ on phase space in the sense that for all semiclassical observables with symbols $a\in C^\infty_{\rm b}(Z)$

$$\lim_{\varepsilon\to 0}\left|\langle\phi^\varepsilon,\,\widehat{a}\,\phi^\varepsilon\rangle-\int_Z a(q,p)\,\rho_{\rm cl}(\mathrm{d}q\,\mathrm{d}p)\right|=0\,. \tag{2.57}$$

The definition is equivalent to saying that the Wigner transform of ϕ^ε converges to $\rho_{\rm cl}$ weakly on test functions in $C^\infty_{\rm b}(Z)$ [LiPa]. An immediate application of Egorov's theorem (cf. [Ro, BoRo] and Section 3.4) yields

$$\lim_{\varepsilon\to 0}\left|\langle\phi^\varepsilon,\,\mathrm{e}^{\mathrm{i}H^\varepsilon_{\rm BO}t/\varepsilon}\,\widehat{a}\,\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm BO}t/\varepsilon}\,\phi^\varepsilon\rangle-\int_Z (a\circ\Phi^t)(q,p)\,\rho_{\rm cl}(\mathrm{d}q\,\mathrm{d}p)\right|=0 \tag{2.58}$$

uniformly on bounded intervals in time, where we recall that Φ^t is the flow generated by (2.49). In (2.58) one can of course shift the time evolution from the observables to the states on both sides and write instead

$$\lim_{\varepsilon\to 0}\left|\langle\phi^\varepsilon_t,\,\widehat{a}\,\phi^\varepsilon_t\rangle-\int_Z a(q,p)\,\rho_{\rm cl}(\mathrm{d}q\,\mathrm{d}p,t)\right|=0\,. \tag{2.59}$$

Here $\phi^\varepsilon_t=\mathrm{e}^{-\mathrm{i}H_{\rm BO}t/\varepsilon}\phi^\varepsilon$ and $\rho_{\rm cl}(\mathrm{d}q\,\mathrm{d}p,t)=\big(\rho_{\rm cl}\circ\Phi^{-t}\big)(\mathrm{d}q\,\mathrm{d}p)$ is the initial distribution $\rho_{\rm cl}(\mathrm{d}q\,\mathrm{d}p)$ transported along the classical flow. Thus with respect to certain type of experiments the system described by the wave function ϕ^ε_t behaves like a classical system.

For a molecular system the object of real interest is the left hand side of (2.59) with ϕ^ε_t replaced by the solution ψ^ε_t of the full Schrödinger equation and $\widehat{a}=:a^\varepsilon_{\rm BO}$ as acting on $L^2(\mathbb{R}^d)$ replaced by $\widehat{a}\otimes\mathbf{1}$ as acting on $\mathcal{H}$. In order to compare the expectations of $a^\varepsilon_{\rm BO}$ with the expectations of $\widehat{a}\otimes\mathbf{1}$, we need the following proposition.

Proposition 2.16. *In addition to the assumptions of Theorem 2.14 let $a\in C^\infty_{\rm b}(Z)$ with*

$$\int\mathrm{d}\xi\,\sup_{x\in\mathbb{R}^d}|\xi|\,|(\mathcal{F}_{(2)}a)(x,\xi)|\,<\infty\,, \tag{2.60}$$

where $\mathcal{F}_{(2)}$ denotes Fourier transformation in the second argument. Then there is a constant $C<\infty$ such that

$$\|(\widehat{a}\otimes\mathbf{1}\,-\,\mathcal{U}^*\,\widehat{a}\,\mathcal{U})\;\mathbf{1}_{\Lambda-\delta}\,P_*\,\|\;\le\;C\,\varepsilon\,.$$

We postpone the proof of Proposition 2.16 to the end of this section. With its help we obtain the semiclassical limit for the nuclei as governed by the full Hamiltonian.

Corollary 2.17. *Let Γ and I be as in Theorem 2.14. Let $\psi^\varepsilon\in\mathcal{H}$ such that (2.57) is satisfied for $\phi^\varepsilon:=\mathcal{U}P_*\psi^\varepsilon$ for some $\rho_{\rm cl}$ with $\mathrm{supp}\rho_{\rm cl}\subset\Gamma-\alpha$. Let $\psi^\varepsilon_t=\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}\psi^\varepsilon$ then for all $a\in C^\infty_{\rm b}(Z)$ which satisfy (2.60)*

$$\lim_{\varepsilon\to 0}\left|\langle\psi^\varepsilon_t,\,(\widehat{a}\otimes\mathbf{1})\,\psi^\varepsilon_t\rangle-\int_Z a(q,p)\,\rho_{\rm cl}(\mathrm{d}q\,\mathrm{d}p,t)\right|=0 \tag{2.61}$$

uniformly for $t\in I$.

Translated to the language of Wigner measures Corollary 2.17 states the following. Let us define the marginal Wigner transform for the nuclei as

$$W^{\varepsilon}_{\mathrm{nuc}}(\psi^{\varepsilon}_t)(q,p) := (2\pi)^{-d} \int_{\mathbb{R}^d} \mathrm{d}x\, \mathrm{e}^{\mathrm{i}x\cdot p}\, \langle \psi^{\varepsilon *}_t(q+\varepsilon x/2), \psi^{\varepsilon}_t(q-\varepsilon x/2)\rangle_{\mathcal{H}_{\mathrm{e}}}\,.$$

Then, whenever $W^{\varepsilon}_{\mathrm{nuc}}(P_*\psi^{\varepsilon}_0)(q,p)\,\mathrm{d}q\,\mathrm{d}p$ converges weakly to some probability measure $\rho_{\mathrm{cl}}(\mathrm{d}q\,\mathrm{d}p)$, $W^{\varepsilon}_{\mathrm{nuc}}(P_*\psi^{\varepsilon}_t)(q,p)\,\mathrm{d}q\,\mathrm{d}p$ converges weakly to $(\rho_{\mathrm{cl}}\circ \Phi^{-t})(\mathrm{d}q\,\mathrm{d}p)$.

Corollary 2.17 follows by applying first Proposition 2.16 and then Theorem 2.14 to the left hand side in the difference (2.61), where we note that $\lim_{\varepsilon\to 0}\|(1-P^{\alpha}_{\Gamma})\psi^{\varepsilon}\| = 0$ and thus also $\lim_{\varepsilon\to 0}\|(1-P_{\Lambda-\delta'})\psi^{\varepsilon}_t\| = 0$ for any $\delta' < \delta$. This yields the left hand side of (2.58) and thus (2.61).

We mention some standard examples of initial wave functions ϕ^{ε} of the nuclei which approximate certain classical distributions. The initial wave function for the full system is, as before, recovered as $\psi^{\varepsilon} = \mathcal{U}^*\phi^{\varepsilon} = \phi^{\varepsilon}(x)\chi(x)$. In these examples one regains some control on the rate of convergence with respect to ε which was lost in (2.57).

(i) Wave packets tracking a classical trajectory.

For $\phi \in L^2(\mathbb{R}^d)$ let

$$\phi^{\varepsilon}_{q_0,p_0}(x) = \varepsilon^{-d/4}\,\mathrm{e}^{-\mathrm{i}(p_0\cdot(x-q_0))/\varepsilon}\phi\big(\frac{x-q_0}{\sqrt{\varepsilon}}\big)\,.$$

Then $|\phi^{\varepsilon}_{q_0,p_0}(x)|^2$ is sharply peaked at q_0 for ε small and its ε-scaled Fourier transform is sharply peaked at p_0. Thus one expects that the corresponding classical distribution is given by $\delta(q-q_0)\delta(p-p_0)\,\mathrm{d}q\,\mathrm{d}p$. As was shown, e.g. in [TeSp], this is indeed true for $\phi \in L^2(\mathbb{R}^d)$ such that $\phi, |x|\phi, \widehat{\phi}, |p|\widehat{\phi} \in L^1(\mathbb{R}^d)$, where $\widehat{\phi}$ denotes the Fourier transform of ϕ. Then Corollary 2.17 holds with (2.61) replaced by

$$\begin{aligned} &|\langle \psi^{\varepsilon}_t,\, (\widehat{a}\otimes \mathbf{1})\,\psi^{\varepsilon}_t\rangle - a(q(t),p(t))\,| \\ &= \mathcal{O}(\sqrt{\varepsilon})\,\Big(\|\phi\|^2_{L^2} + \|\phi\|_{L^1}\,\||p|\widehat{\phi}\|_{L^1} + \||x|\phi\|_{L^1}\,\|\widehat{\phi}\|_{L^1}\Big)\,, \end{aligned} \tag{2.62}$$

where $(q(t),p(t))$ is the solution of the classical dynamics with initial condition (q_0,p_0). Equation (2.62) generalizes Hagedorn's first order result in [Ha$_1$] to a larger class of localized wave functions.

(ii) Either sharp momentum or sharp position.

For $\phi \in L^2(\mathbb{R}^d)$ let

$$\widehat{\phi}^{\varepsilon}_{p_0}(p) = \widehat{\phi}(p-p_0/\varepsilon)\,,$$

where $\widehat{\ }$ denotes the ε-scaled Fourier transformation, then the corresponding classical distribution is $\rho_{\mathrm{cl}}(\mathrm{d}q\,\mathrm{d}p) = \delta(p-p_0)|\phi(q)|^2\,\mathrm{d}q\,\mathrm{d}p$. Note that the absolute value of ϕ does not depend on ε in that case. Equivalently one defines

$$\phi^{\varepsilon}_{q_0}(x) = \varepsilon^{-d/2}\phi\big(\frac{x-q_0}{\varepsilon}\big)$$

and obtains $\rho_{\rm cl}(\mathrm{d}q\,\mathrm{d}p) = \delta(q-q_0)|\widehat{\phi}(p)|^2\,\mathrm{d}q\,\mathrm{d}p$. In both cases one finds that the difference in (2.61) is bounded a constant times either $\varepsilon\big(\|\phi\|^2_{L^2} + \|\phi\|_{L^1}\||p|\widehat{\phi}\|_{L^1}\big)$ for $\phi^{\varepsilon}_{p_0}$ or $\varepsilon\big(\|\phi\|^2_{L^2} + \||x|\phi\|_{L^1}\|\widehat{\phi}\|_{L^1}\big)$ for $\phi^{\varepsilon}_{q_0}$.

(iii) WKB wave functions.

For $f \in L^2(\mathbb{R}^d)$ and $S \in C^1(\mathbb{R}^d)$ both real valued let

$$\phi^{\varepsilon}(x) = f(x)\,\mathrm{e}^{\,\mathrm{i}S(x)/\varepsilon}\,,$$

then $\rho_{\rm cl}(\mathrm{d}q\,\mathrm{d}p) = f^2(q)\,\delta(p-\nabla S(q))\,\mathrm{d}q\,\mathrm{d}p$. In this case one expects that (2.61) is bounded as $\sqrt{\varepsilon}$, which has been shown in [TeSp] for a smaller set of test functions.

Proof (of Proposition 2.16). For the following calculations we continue $\chi(\cdot) \in C^{\infty}_{\rm b}(\Lambda, \mathcal{H}_{\rm e})$ arbitrarily to a function $\chi(\cdot) \in C^{\infty}_{\rm b}(\mathbb{R}^n, \mathcal{H}_{\rm e})$ by possibly modifying it on $\Lambda \setminus (\Lambda - \delta/2)$. For ϕ in a dense subset of $L^2(\Lambda-\delta)$ and $x \in \Lambda - \delta/2$, by making the substitutions $\widetilde{k} = \varepsilon k$ and $\widetilde{y} = (y-x)/\varepsilon$ and using Taylor expansion with rest, we have:

$$\begin{aligned}
&\big(\big(a^{\mathrm{W},\varepsilon} \otimes \mathbf{1}\big)\,\phi\chi\big)\,(x) = \\
&\quad = (2\pi)^{-n} \int \mathrm{d}y\,\mathrm{d}k\, a\left(\frac{x+y}{2}, \varepsilon k\right) \mathrm{e}^{-\mathrm{i}(x-y)\cdot k}\,\phi(y)\chi(y) \\
&\quad = (2\pi)^{-n} \int \mathrm{d}\widetilde{y}\,\widehat{a}^{(2)}\left(x + \frac{\varepsilon}{2}\widetilde{y}, -\widetilde{y}\right)\,\phi(x+\varepsilon\widetilde{y})\,\chi(x) \\
&\qquad + \varepsilon\,(2\pi)^{-n} \int \mathrm{d}\widetilde{y}\,\widehat{a}^{(2)}\left(x + \frac{\varepsilon}{2}\widetilde{y}, -\widetilde{y}\right)\,\phi(x+\varepsilon\widetilde{y})\,\widetilde{y}\cdot\big(\nabla_x\chi\big)(f(x,\varepsilon\widetilde{y})) \\
&\quad = \big(\mathcal{U}^*\,a^{\mathrm{W},\varepsilon}\,\mathcal{U}\,\phi\chi\big)\,(x) \,+\, R^{\varepsilon}\,. \qquad (2.63)
\end{aligned}$$

From (2.63) we conclude that

$$\big\|\big(\mathbf{1}_{\Lambda-\delta/2}(\cdot)\otimes\mathbf{1}\big)\,\big(a^{\mathrm{W},\varepsilon}\otimes\mathbf{1} - \mathcal{U}^*\,a^{\mathrm{W},\varepsilon}\,\mathcal{U}\big)\,P_{\Lambda-\delta}\big\| \le \|R^{\varepsilon}\|\,.$$

Since

$$\begin{aligned}
&\big\|\big(\mathbf{1} - \mathbf{1}_{\Lambda-\delta/2}(\cdot)\otimes\mathbf{1}\big)\,\big(a^{\mathrm{W},\varepsilon}\otimes\mathbf{1} - \mathcal{U}^*\,a^{\mathrm{W},\varepsilon}\,\mathcal{U}\big)\,P_{\Lambda-\delta}\big\| \\
&= \big\|\big(\mathbf{1} - \mathbf{1}_{\Lambda-\delta/2}(\cdot)\otimes\mathbf{1}\big)\,\big(a^{\mathrm{W},\varepsilon}\otimes\mathbf{1} - \mathcal{U}^*\,a^{\mathrm{W},\varepsilon}\,\mathcal{U}\big)\,\big(\mathbf{1}_{\Lambda-\delta}(\cdot)\otimes\mathbf{1}\big)P_{\Lambda-\delta}\big\| \\
&= O(\varepsilon^n)
\end{aligned}$$

for arbitrary n, Proposition 2.16 follows by showing that R^{ε} is of order ε:

$$\begin{aligned}
\|R^{\varepsilon}\| &\le \varepsilon\,(2\pi)^{-n} \int \mathrm{d}\widetilde{y}\,\Big\|\widehat{a}^{(2)}\left(\cdot + \frac{\varepsilon}{2}\widetilde{y}, -\widetilde{y}\right)\,\phi(\cdot+\varepsilon\widetilde{y})\,\widetilde{y}\cdot\big(\nabla_x\chi\big)(f(\cdot,\varepsilon\widetilde{y}))\Big\|_{\mathcal{H}} \\
&\le \varepsilon\,(2\pi)^{-n} \sup_{x\in\mathbb{R}^n} \|(\nabla_x\chi)(x)\|_{\mathcal{H}_{\rm e}}
\end{aligned}$$

$$\times \int \mathrm{d}\widetilde{y} \left\| \widehat{a}^{(2)}\left(\cdot + \frac{\varepsilon}{2}\widetilde{y}, -\widetilde{y}\right) |\widetilde{y}|\, \phi(\cdot + \varepsilon\widetilde{y}) \right\|_{L^2(\mathbb{R}^n)}$$

$$\leq \varepsilon\, C\, \|\phi\|_{L^2(\mathbb{R}^n)} \int \mathrm{d}\widetilde{y} \sup_{x\in\mathbb{R}^n} |\widetilde{y}|\, |\widehat{a}^{(2)}(x,\widetilde{y})|$$

$$= \varepsilon\, \widetilde{C}\, \|\phi\chi\|_{\mathcal{H}}\,.$$

□

2.3.4 Born-Oppenheimer approximation in a magnetic field and Berry's connection

In this section we exemplify the physical importance of the correction $\mathcal{A}$ in the effective Born-Oppenheimer Hamiltonian (2.46) in a simple but drastic example. For a more detailed discussion of the geometric origin of Berry's connection we refer to Section 3.4.2.

Within a naive Born-Oppenheimer approximation, where Berry's connection is neglected, an external magnetic field would act on the nuclei as if they were naked charges. Clearly this would not describe the physics properly, since a neutral molecule moving in an external magnetic field would not be deflected by the Lorentz force. This was first observed by Schmelcher et al. [SCM], who therefore introduced a screened Born-Oppenheimer approximation. Mead and Yin [Me, YiMe] realized that the screening of the nuclei is, in a proper Born-Oppenheimer approximation, provided by the Berry connection: in such a case the geometric vector potential $\mathcal{A}$ approximately cancels the vector potential A of the external magnetic field. This can be easily checked for an atom in a constant magnetic field by direct computation, where the cancellation is indeed exact. The following is taken from the very recommendable lecture notes of Resta [Re] on Berry's phase in physics.

Let $A(x) = \frac{1}{2}B \times x$ be the vector potential of a constant magnetic field B. For a hydrogen atom, i.e. a molecule which contains only one nucleus and one electron, the electronic Hamiltonian is given through

$$H_{\mathrm{e}}(x) = \frac{1}{2}\left(-\mathrm{i}\nabla_y - \frac{1}{2}B \times y\right)^2 + V(|x-y|)\,,$$

where $x, y \in \mathbb{R}^3$. Let $\chi_0(0,y) \subset \mathcal{H}_{\mathrm{e}}$ be the ground state of $H_{\mathrm{e}}(0)$, i.e. the ground state for the system where the nucleus is at the origin. Then the ground state at a different location $x \in \mathbb{R}^3$ is obtained through a magnetic translation,

$$\chi_0(x,y) = \mathrm{e}^{\frac{\mathrm{i}}{2}y\cdot B\times x}\, \chi_0(0, y-x) = \mathrm{e}^{\frac{\mathrm{i}}{2}x\cdot y\times B}\, \chi_0(0,y-x)\,.$$

Thus one finds for the Berry connection

$$\begin{aligned}\mathcal{A}(x) &= \mathrm{i}\langle \chi_0(x,y), \nabla_x \chi_0(x,y)\rangle_{\mathcal{H}_{\mathrm{e}}} \\ &= \tfrac{1}{2}B \times \langle \chi_0(x,y),\, y\, \chi_0(x,y)\rangle_{\mathcal{H}_{\mathrm{e}}} - \langle \chi_0(0,y-x),\, \nabla_y \chi_0(0,y-x)\rangle_{\mathcal{H}_{\mathrm{e}}} \\ &= \tfrac{1}{2}B \times x\,,\end{aligned}$$

where one uses the symmetries of the ground state wave function. Hence $\mathcal{A} = A$ and the Berry connection cancels exactly the magnetic potential in the correct Born-Oppenheimer Hamiltonian (2.46).

2.4 Constrained quantum motion

It is a classical problem of mathematical physics to determine effective equations of motion for a system which is constrained to a smooth submanifold of configuration space through strong external forces. The question can be asked for classical as well as for quantum systems. The classical problem was rigorously studied by Rubin and Ungar [RuUn] and later by Takens [Ta]. Under suitable conditions the problem of constrained motion for classical Hamiltonian systems can be formulated as an classical adiabatic problem, e.g. [LoMe]. A detailed treatment of the classical problem from the point of view of weak convergence is given in the book of Bornemann [Bor]. In a recent work of Froese and Herbst [FrHe] the authors discuss and compare the classical and the quantum case.

In this section we reconsider the quantum mechanical problem from the point of view of adiabatic decoupling. Usually, cf. [Bor, FrHe], the limit of strong confinement is realized through dilations in the normal direction of the constrained manifold. On the level of classical mechanics one can equivalently dilate the tangential direction by the inverse factor and obtains, up to a total scaling of space-time, the same limit dynamics. However, for the quantum mechanical problem the two approaches are not equivalent anymore. We shall argue that the physical problem is best modelled by the second approach, i.e. by scaling the tangential direction. Formulated in this way, the problem is similar to the Born-Oppenheimer approximation and can be solved using exactly the same methods. The same observation was made independently by Ben Abdallah and Mehats, who announced a result on the semiclassical limit in partially confining potentials based on Wigner measures [BeMe].

2.4.1 The classical problem

Consider a particle or a system of particles with configuration space $\mathbb{R}^{n+m}$ whose classical motion is governed by a Hamiltonian function

$$H^\varepsilon(q,p) = \frac{1}{2}\,p^2 + V(q) + W^\varepsilon(q) \tag{2.64}$$

on phase space $\mathbb{R}^{2(n+m)}$, where $W^\varepsilon(q)$ constrains the motion to near some submanifold $\Sigma \subset \mathbb{R}^{n+m}$ of configuration space. By constraining one means that $W^\varepsilon(q)$ vanishes on Σ and rapidly increases away from Σ. In order to avoid complications coming from nontrivial geometry, which would cloud the simple ideas behind the following, we restrict ourselves to the case where

$\Sigma = \mathbb{R}^m$ is a subspace of configuration space. We split $q = (x, y) \in \mathbb{R}^n_x \times \mathbb{R}^m_y$ and write the potentials as

$$W^\varepsilon(q) = W(x, y/\varepsilon) \in [0, \infty)\,, \quad V(q) = V(x)\,, \tag{2.65}$$

where all dependence on y in the external potentials is absorbed into the definition of W. The conditions

$$W(x, y) = 0 \Leftrightarrow y = 0 \quad \text{and} \quad \lim_{|y|\to\infty} W(x, y) = \infty$$

express the fact that W is confining: in the limit $\varepsilon \to 0$ for every point (x, y) with $y \neq 0$ the potential energy $W^\varepsilon(x, y) = W(x, y/\varepsilon)$ will eventually tend to plus infinity as ε decreases.

The heuristic picture is as follows. Assume that the initial configuration q_0 lies on the constraint manifold Σ, i.e. $y_0 = 0$ in our setting. For such initial conditions and for small ε, the solution $(q^\varepsilon(t), p^\varepsilon(t))$ of the classical equations of motion

$$\dot{q} = p \qquad \dot{p} = -\nabla V(q) - \nabla W^\varepsilon(q) \tag{2.66}$$

remains near Σ for all times by conservation of energy. The smaller ε is, the smaller are the maximal deviations from Σ. Hence $(q^\varepsilon(t), p^\varepsilon(t))$ converges in the limit $\varepsilon \to 0$ to some limiting trajectory which remains completely on Σ. The interesting question is now whether there are effective equations of motion for a reduced system, i.e. for a system with configuration space Σ, which have as solutions exactly the limiting solutions of the full system, and how they look.

This problem has been attacked on a rigorous level by many authors under different names and with different emphasis. Recent results including reviews of the field can be found in [FrHe], who formulate the question of "realizing holonomic constraints", and in [Bor], who relies on weak convergence instead of asymptotic expansions. Since it is instructive to compare the classical and the quantum mechanical results, we briefly explain a simple version of the classical results going back to Rubin and Ungar [RuUn] and Takens [Tak].

Assume that W is quadratic in the constraining direction, i.e. that

$$W^\varepsilon(x, y) = \frac{1}{2\varepsilon^2}\,\langle y, A(x)\,y\rangle_{\mathbb{R}^m}\,, \tag{2.67}$$

where $A(x)$ is a positive definite $m \times m$-matrix with smooth coefficients. Let $\{\omega^2_\alpha(x)\}^k_{\alpha=1}$ be the set of eigenvalues of $A(x)$ with corresponding spectral projections $P_\alpha(x)$ and assume that all $\omega^2_\alpha(x)$ have constant multiplicity as x varies. In the simplest setup one assumes that the initial condition (q_0, p_0) lies on Σ, i.e. that $q_0 = (x_0, 0)$. The normal component η_0 of the initial velocity $p_0 = (\xi_0, \eta_0)$ plays a crucial role in the effective dynamics through the action variables for the oscillatory normal motion defined as

$$I_\alpha(q_0, p_0) = \frac{\langle \eta_0, P_\alpha(x_0)\,\eta_0\rangle_{\mathbb{R}^m}}{2\omega_\alpha(x_0)}\,.$$

The I_α's are classical adiabatic invariants, cf. [LoMe], i.e. they are approximate constants of motion. Their role is to define the effective potential for the limiting dynamics on Σ through the total energy stored in the fast oscillations,

$$V_{\text{eff}}(x) = V(x) + \sum_{\alpha=1}^{k} I_\alpha \, \omega_\alpha(x) \,. \tag{2.68}$$

Here $I_\alpha \omega_\alpha(x)$ is the energy stored in the α^{th} oscillator. The following statement is included, e.g., in the results obtained in [FrHe].

Theorem 2.18. *Let $(q^\varepsilon(t), p^\varepsilon(t))$ be the solution of (2.66) with initial condition (q_0, p_0) satisfying $y_0 = 0$. Then the limits $x^0(t) = \lim_{\varepsilon\to 0} x^\varepsilon(t)$ and $\xi^0(t) = \lim_{\varepsilon\to 0} \xi^\varepsilon(t)$ exist pointwise for all $t \in \mathbb{R}$ and uniformly on any bounded interval in time. Furthermore $(x^0(t), \xi^0(t))$ is given through the unique solution of the effective equations of motion governed by the Hamiltonian*

$$H_{\text{eff}}(x, \xi) = \frac{1}{2}\, \xi^2 + V_{\text{eff}}(x)$$

with initial condition (x_0, ξ_0).

Remark 2.19. It should be noted that in the classical results the confining potential is usually taken to be of the form

$$W^\varepsilon(x, y) = \frac{1}{\varepsilon^2}\, W(x, y) \,, \tag{2.69}$$

i.e. the limit of strong confinement is not realized through dilations in the normal direction, but through a scaling of the size of the potential away from Σ. As a consequence the limiting behavior is completely determined by the quadratic part of $W(x, \cdot)$, more precisely by the Hessian $\nabla_y^{(2)} W(x, 0)$ on Σ. However, formulating the problem as in (2.65) seems more natural and contains more general limiting behavior, at least in the quantum case. Moreover, formally (2.69) can be understood as the dilation of an ε dependent potential given through the Taylor expansion of W, i.e.

$$\frac{1}{\varepsilon^2}\, W(x, y) = \widetilde{W}^\varepsilon(x, y/\varepsilon)$$

with

$$\widetilde{W}(x, y) = \sum_{j=2}^{\infty} \frac{\varepsilon^{j-2}\, y^j}{j!}\, W^{(j)}(x, 0) \,,$$

where we assumed $m = 1$ to keep notation simple. This also explains why the Hessian $\nabla_y^{(2)} W(x, 0)$ alone determines the limit dynamics when the scaling (2.69) is used: higher order terms in the Taylor expansion of W enter at higher order with respect to an expansion in ε. In the language of the quantum mechanical result, only the quadratic part of W enters the principal symbol of the relevant Hamiltonian. ♢

2.4.2 A quantum mechanical result

We now come to the analogous quantum mechanical problem, which is usually taken to be the limit $\varepsilon \to 0$ for the dynamics generated by the Hamiltonian

$$H^{\varepsilon}_{\mathrm{hol}} = -\frac{1}{2}\,\Delta_x - \frac{1}{2}\,\Delta_y + V(x) + W(x, y/\varepsilon) \tag{2.70}$$

acting on $L^2(\mathbb{R}^{n+m})$. This problem was studied for example in [FrHe] in the context of understanding holonomic constraints in quantum mechanics. The main problem one encounters in this approach is the divergence in energy for any initial condition: the smaller ε is, the better the initial wave function must be localized on Σ in order to keep the potential energy bounded, which leads to a divergence in kinetic energy.

From a physical point of view such a limit seems therefore somewhat unnatural. In actual experiments there is always a natural boundary beyond which the particles can not be further localized. Hence we suggest to put the question differently. Instead of the limit of strong constraining forces we consider the limit of weak forces in the non-constraining direction. Indeed, a simple argument shows that both limits are equivalent, up to a rescaling of space-time, in the case of classical mechanics.

More precisely, instead of using macroscopic coordinates as in

$$H^{\varepsilon}(q,p) = \frac{1}{2}\,p^2 + V(x) + W(x, y/\varepsilon)\,,$$

i.e. (2.64), consider the classical Hamiltonian in microscopic coordinates

$$\widetilde{H}^{\varepsilon}(\tilde{q},\tilde{p}) = \frac{1}{2}\,\tilde{p}^2 + V(\varepsilon\tilde{x}) + W(\varepsilon\tilde{x},\tilde{y})\,,$$

where now the potentials are slowly varying in the tangential direction of Σ, instead of strongly confining in the normal direction. As always, macroscopic and microscopic space-time coordinates are related through $q = \varepsilon\tilde{q}$ and $t = \varepsilon\tilde{t}$. If $(\tilde{q}^{\varepsilon}(\tilde{t}), \tilde{p}^{\varepsilon}(\tilde{t}))$ is a solution to the equations of motion generated by $\widetilde{H}^{\varepsilon}(\tilde{q},\tilde{p})$ then one can check by direct computation that

$$\big(q(t), p\,(t)\big) := \left(\varepsilon\tilde{q}\left(\frac{t}{\varepsilon}\right), \tilde{p}\left(\frac{t}{\varepsilon}\right)\right)$$

is a solution of the equations of motion generated by $H^{\varepsilon}(q,p)$. Hence the motion generated by $\widetilde{H}^{\varepsilon}(\tilde{q},\tilde{p})$ is related to the motion generated by $H^{\varepsilon}(q,p)$ through a rescaling of space-time and the limit $\varepsilon \to 0$ can be studied equally well in microscopic or macroscopic units.

In the quantum mechanical case the limiting behavior is not independent of the scaling anymore. While for the classical problem it makes no difference whether one fixes the microscopic or the macroscopic scale and makes the other one ε-dependent, in quantum mechanics there is an a priori microscopic

scale defined through $\hbar$. As a consequence it makes a qualitative difference, whether one scales this microscopic or a corresponding macroscopic scale with ε. As argued above, from a physical point of view it seems more natural to keep the microscopic scale—the scale of the constraining potential—fixed, and to consider weak tangential forces to Σ and thus to define the macroscopic scale through ε.

In the special case of constraining to a subspace this leads us to consider the Hamiltonian

$$\widetilde{H}^\varepsilon = -\frac{1}{2}\,\Delta_{\tilde{x}} - \frac{1}{2}\,\Delta_{\tilde{y}} + V(\varepsilon\tilde{x}) + W(\varepsilon\tilde{x},\tilde{y}) \tag{2.71}$$

as our starting Hamiltonian, where we use microscopic coordinates. Of course one expects a sensible limiting behavior on the constraint manifold only on the macroscopic level and thus substitutes $x = \varepsilon\tilde{x}$. Then (2.71) takes the Born-Oppenheimer form

$$H^\varepsilon = -\frac{\varepsilon^2}{2}\,\Delta_x - \frac{1}{2}\,\Delta_{\tilde{y}} + V(x) + W(x,\tilde{y}) =: -\frac{\varepsilon^2}{2}\,\Delta_x + H_{\mathrm{e}}(x)\,, \tag{2.72}$$

and one can directly apply the results of Section 2.3 in order to cover very general potentials W and V.

Remark 2.20. Note that $H^\varepsilon_{\mathrm{hol}}$ defined in (2.70) and H^ε defined in (2.72) are not related through a rescaling of space-time, as it is true in classical mechanics. Thus on the quantum level one has two different scaling problems to consider. The situation is similar to the one encountered in Section 6.3 for the massless Nelson model. There it turns out that classically one can equivalently consider the limit of fast photons or the limit if slow particles. In the corresponding quantum mechanical model the two limits are not equivalent anymore. ♢

For sake of comparison let us restrict ourselves again to the case of quadratic confining potential as in (2.67). Then $H_{\mathrm{e}}(x)$ is just the Hamiltonian of the harmonic oscillator plus an x-dependent energy shift,

$$H_{\mathrm{e}}(x) = -\frac{1}{2}\,\Delta_{\tilde{y}} + \frac{1}{2}\,\langle\tilde{y}, A(x)\,\tilde{y}\rangle_{\mathbb{R}^m} + V(x) \tag{2.73}$$

with x-independent domain $H^2(\mathbb{R}^m)\cap D(\tilde{y}^2)$. The spectrum of $H_{\mathrm{e}}(x)$ is purely discrete and given through

$$E_\gamma(x) = V(x) + \sum_{\alpha=1}^{k} (\gamma_\alpha + \tfrac{1}{2})\omega_\alpha(x)\,, \qquad \gamma \in \mathbb{N}^k\,.$$

Fix a $\gamma \in \mathbb{N}^k$ such that the corresponding eigenvalue $E_\gamma(x)$ is bounded and globally separated by a gap, i.e. satisfies condition **Gap** of Section 2.3, and, for simplicity, assume that $E_\gamma(x)$ is nondegenerate. Denote by $P_\gamma(x)$ the projection on the corresponding eigenspace of $H_{\mathrm{e}}(x)$ and let $P_\gamma = \int^{\oplus}_{\mathbb{R}^n} \mathrm{d}x\, P_\gamma(x)$. Then the following result is just a special case of Theorem 2.16.

Theorem 2.21. *Let H^ε be as in (2.72) and (2.73) and $\gamma \in \mathbb{N}^k$ be chosen as explained above. Define*

$$H^\varepsilon_{\text{eff}} = -\frac{\varepsilon^2}{2}\,\Delta_x + V_{\text{eff}}(x)$$

with

$$V_{\text{eff}}(x) = V(x) + E_\gamma(x) = V(x) + \sum_{\alpha=1}^{k} (\gamma_\alpha + \tfrac{1}{2})\,\omega_\alpha(x)\,, \tag{2.74}$$

and let $\mathcal{U}$ be as in Section 2.3. Then there is a constant $C < \infty$ such that

$$\left\| \left(\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} - \mathcal{U}^*\, \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\text{eff}} t/\varepsilon}\, \mathcal{U} \right) P_\gamma \right\|_{\mathcal{L}(H^{2,\varepsilon}\otimes L^2(\mathbb{R}^m),\mathcal{H})} \leq C\varepsilon(1+|t|)\,. \tag{2.75}$$

Note that the results of Section 2.3 and Chapter 4 would allow for a much larger class of confining potentials, for nondegenerate eigenvalues and for higher order corrections to the effective Hamiltonian. However, the very special formulation of Theorem 2.21 allows for a nice comparison with the classical result presented in Section 2.4.1.

2.4.3 Comparison

When the limit of strong confinement is implemented through dilations in the confining direction, there are no finite energy solutions of the problem in the quantum mechanical case. In [FrHe] a comparison of the limit of strong confinement in classical and quantum mechanics was made possible, because the authors considered also the classical problem with ε-dependent initial conditions of diverging energy. On the other hand, by keeping the confining potential fixed and scaling the non-confining direction instead, we were able to consider finite energy solutions also in the quantum mechanical case. As a consequence a comparison with the finite energy solutions in the classical case is now possible.

In the classical case (2.68) as well as in the quantum mechanical case (2.74) the effective potentials guiding the motion on the constrained manifold depend on and are determined by the initial conditions. However, the underlying structure is very different, although the effective potentials have a quite similar appearance.

In quantum dynamics the state space splits into subspaces which are approximately invariant under the time-evolution. The adiabatic invariants are the norms of the wave function projected onto these subspaces, i.e.

$$I_\gamma(\psi_t) := \langle \psi_t,\, P_\gamma \psi_t \rangle \approx I_\gamma(\psi_0)\,.$$

On each subspace the dynamics is generated by a fixed effective Hamiltonian. By linearity of Schrödinger's equation, in a superposition of states from different invariant subspaces each component follows its own effective dynamics.

The different effective potentials corresponding to different eigenvalues are *not* added or superimposed in any way.

In classical mechanics the part of the phase space with configuration on Σ is further foliated into submanifolds with $I_\alpha(x,p) = \text{const.}$ for all α. Since I_α are classical adiabatic invariants, these submanifolds are approximately invariant under the classical flow. On each submanifold there is a corresponding effective potential for the limiting dynamics, which is obtained by *adding* the energies in the fast oscillations as $\sum_\alpha I_\alpha \omega_\alpha(x)$. This is in sharp contrast to the quantum mechanical case described above.

Beyond these simple observations it seems that there is a deeper relation between the classical and quantum mechanical results, which needs to be explored. In the remainder of this section we collect a few observations indicating such a relation.

First of all observe that the possible effective potentials for the quantum motion

$$V^{\mathrm{Q}}_{\mathrm{eff}}(x) = V(x) + \sum_{\alpha=1}^{k} (\gamma_\alpha + \tfrac{1}{2})\, \omega_\alpha(x)$$

are obtained from the classical ones

$$V^{\mathrm{C}}_{\mathrm{eff}}(x) = V(x) + \sum_{\alpha=1}^{k} I_\alpha\, \omega_\alpha(x)$$

by restricting the action variables I_α to integer$+\frac{1}{2}$ multiples of $\hbar$, where the latter was set equal to one. This is just the Bohr-Sommerfeld quantization condition of old quantum theory.

Another interesting relation might be the following. In results on the classical problem where W is not quadratic, there appear so called no-resonance conditions, cf. [Bor]. A resonance of order j occurs when there is a $\gamma \in \mathbb{Z}^k$ with $|\gamma| = j$ such that

$$\sum_{\alpha=1}^{k} \gamma_\alpha\, \omega_\alpha(x) = 0\,.$$

If there are no resonances of any order, it follows that there are no accidental degeneracies of the eigenvalues of the corresponding harmonic oscillator, i.e. all eigenvalue bands $E_\gamma(x)$ of the Hamiltonian $H_{\mathrm{e}}(x)$ are isolated. Indeed, let $\gamma, \gamma' \in \mathbb{N}^k$ with $\gamma \neq \gamma'$, then

$$E_\gamma(x) - E_{\gamma'}(x) = \sum_{\alpha=1}^{k} (\gamma_\alpha - \gamma'_\alpha)\, \omega_\alpha(x) \neq 0\,.$$

In the classical results one typically assumes that there are no resonances of order 1, 2 and 3, where the ω's are, in the general case, the square-roots of the eigenvalues of the Hessian of the confining potential. In our quantum mechanical results resonances of order different from 1 play a priori no role: if

there is an isolated energy band, then the corresponding subspace decouples and states in the subspace are guided by the corresponding effective Hamiltonian. Crossings among other bands, which might be due to resonances, are irrelevant.

On the other hand, the effective dynamics on a band which is locally isolated, but crosses another band at some submanifold of configuration space, might break down at the crossing manifold, depending on the type of crossing. However, the results of Chapter 6 on adiabatic decoupling without gap, cf. also [AvEl$_1$, Bor], suggest that in the case where $H_{\mathrm{e}}(x)$ is the Hamiltonian of an harmonic oscillator, accidental eigenvalue crossings can be ignored, since the corresponding spectral projections can always be continued smoothly through the crossings. And, as a matter of fact, also the classical result for the harmonic potential can do without assuming the non-resonance condition [FrHe]. Hence it remains to be explored what exactly is the connection between the no-resonances condition (and a related condition on the existence of a smooth spectral decomposition of the Hessian appearing in [Bor]) for the classical results and the condition that a smooth spectral decomposition of $H_{\mathrm{e}}(x)$ should exists, which would appear in a general quantum mechanical result based on adiabatic decoupling without gap.

3 Space-adiabatic perturbation theory

This chapter contains the general framework of space-adiabatic perturbation theory. As explained in the introduction, even first order space-adiabatic theory can, in general, not be based on the methods developed for the time-adiabatic setting and for perturbation of fibered Hamiltonians.

The natural mathematical framework for space-adiabatic theory is that of pseudodifferential operators with operator-valued symbols. Readers who are not familiar with the Weyl calculus can find a short review of the results we will use in Appendix A.

We emphasize that the results presented here are not aimed at most possible generality. Instead we try to find a balance between making no unnecessarily restrictive assumptions and not clouding the underlying structure of the arguments by technicalities at the present stage of our enterprize. It is shown in Chapter 4 and Chapter 5 how to generalize respectively modify the theory in order to cover also those applications from physics, for which the assumptions of the present chapter are not satisfied. The content of this chapter is mainly based on Panati, Spohn and Teufel [PST_1].

We now come to the general setup for space-adiabatic perturbation theory. As indicated already in Equation 1.1 in the introduction, there are three structural ingredients for the theory to be applicable.

(i) The state space of the system decomposes as

$$\mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathcal{H}_{\mathrm{f}} = L^2(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}}) \,,$$

where $L^2(\mathbb{R}^d)$ is the state space of the *slow degrees of freedom* and $\mathcal{H}_{\mathrm{f}}$ is an arbitrary separable Hilbert space, the state space for the *fast degrees of freedom*. The classical phase space of the slow degrees of freedom is thus $T^*\mathbb{R}^d = \mathbb{R}^{2d}$ and points in phase space are denoted by $z = (q, p) \in \mathbb{R}^{2d}$.

(ii) The Hamiltonian $\widehat{H}$ generating the time-evolution of states is given as the Weyl quantization of a semiclassical symbol $H \in S^m_\rho(\varepsilon, \mathcal{L}(\mathcal{H}_{\mathrm{f}}))$,

$$H(\varepsilon, z) \asymp \sum_{j=0}^{\infty} \varepsilon^j \, H_j(z) \,,$$

with values in the bounded self-adjoint operators on $\mathcal{H}_{\mathrm{f}}$.

S. Teufel: LNM 1821, pp. 71–104, 2003.

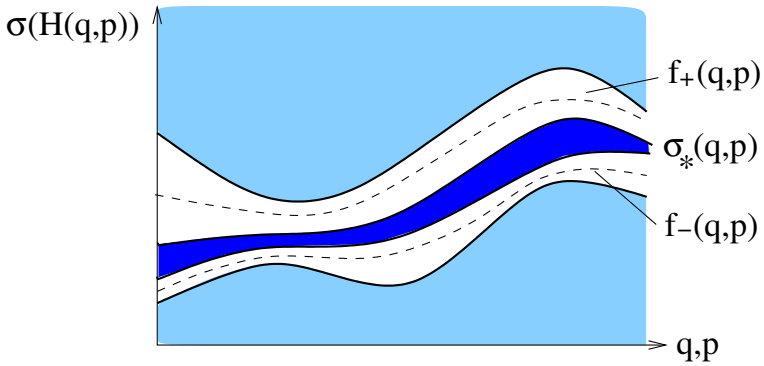

Fig. 3.1. Spectrum which is isolated by a gap locally in phase space $\mathbb{R}^{2d}$.

(iii) The principal symbol $H_0(z)$ of $H(\varepsilon, z)$ has an pointwise isolated part of the spectrum:

Condition (Gap)$_\gamma$. *For any $z \in \mathbb{R}^{2d}$ the spectrum $\sigma(z)$ of $H_0(z) \in \mathcal{L}(\mathcal{H}_\mathrm{f})$ contains a relevant subset $\sigma_*(z)$ which is uniformly separated from the remainder $\sigma(z) \setminus \sigma_*(z)$ by a gap. More precisely there are two continuous functions $f_\pm : \mathbb{R}^{2d} \to \mathbb{R}$ with $f_- \leq f_+$ such that:*

(G1) for every $z \in \mathbb{R}^{2d}$ the spectral component $\sigma_*(z)$ is entirely contained in the interval $I(z) := [f_-(z), f_+(z)]$;

(G2) the distance between $\sigma(z) \setminus \sigma_*(z)$ and the interval $I(z)$ is uniformly bounded away from zero and increasing for large momenta, i.e.

$$\mathrm{dist}\big(\sigma(z) \setminus \sigma_*(z), I(z)\big) \geq C_\mathrm{g} \langle p \rangle^\gamma \, ;$$

(G3) the width of the interval $I(z)$ is uniformly bounded, i.e.

$$\sup_{z \in \mathbb{R}^{2d}} |f_+(z) - f_-(z)| \leq C_\mathrm{d} < \infty \, .$$

We already encountered several relevant physical systems which display this general structure. The Dirac Hamiltonian (1.52) discussed in Section 1.2 is probably the simplest example which is the quantization of a bounded-operator-valued symbol. Clearly also perturbations of fibered Hamiltonians as discussed in Chapter 2 fall into the general framework. However, the examples discussed there, namely the molecular Hamiltonian and the Hamiltonian for constrained quantum motion have symbols with values in the unbounded operators. The theory to be developed in this chapter applies in principle also to this case with minor technical modifications. These modifications are, among more serious ones, discussed in Chapter 5, where the problem of the Bloch electron, i.e. a particle in a periodic potential with a slowly varying non-periodic perturbation, is treated.

At the risk of redundancy we shortly map out again the strategy of space-adiabatic perturbation theory. Each of the following steps corresponds to a section in this chapter.

(i) **Almost invariant subspace.** As the first step one constructs an orthogonal projection Π^ε, which is associated with the isolated spectral band σ_*, such that the subspace $\Pi^\varepsilon\mathcal{H}$ of the full Hilbert space $\mathcal{H}$ is approximately invariant under the time-evolution generated by $\widehat{H}$. By "approximately" we always mean "up to errors which are small when ε is small". In case of the Dirac equation $\Pi^\varepsilon L^2(\mathbb{R}^3, \mathbb{C}^4)$ would be either the electronic or the positronic subspace and both of them are invariant under the time-evolution up to errors smaller than any power of ε.

(ii) **Mapping to a reference space.** We aim at a simple description of the dynamics inside the almost invariant subspace $\Pi^\varepsilon\mathcal{H}$. However, since $\Pi^\varepsilon\mathcal{H}$ is not easy to characterize, we construct a unitary operator U^ε, which maps the "complicated" and ε-dependent subspace $\Pi^\varepsilon\mathcal{H}$ of the large Hilbert space $\mathcal{H}$ to a "simpler" reference space $\mathcal{K}$. $\mathcal{K}$ is chosen in order to best reflect the physics of the reduced system. In the Dirac example the natural wave functions for the description of electrons are $\mathbb{C}^2$-valued functions. Hence the reference space suggested by the physics would be $L^2(\mathbb{R}^3, \mathbb{C}^2)$, being "simpler" than $\Pi^\varepsilon L^2(\mathbb{R}^3, \mathbb{C}^4)$, which contains $\mathbb{C}^4$-valued functions.

(iii) **Effective dynamics.** Since $[\widehat{H}, \Pi^\varepsilon] = \mathcal{O}(\varepsilon^\infty)$ according to the first step, the dynamics for initial conditions inside $\Pi^\varepsilon\mathcal{H}$ is in good approximation generated by the diagonal Hamiltonian $\Pi^\varepsilon\widehat{H}\Pi^\varepsilon$. However, we aim at a description of the dynamics inside the subspace, which allows for an as simple as possible further analysis. This is the reason for mapping the almost invariant subspace $\Pi^\varepsilon\mathcal{H}$ to the reference space $\mathcal{K}$ and for defining the effective Hamiltonian as the diagonal Hamiltonian mapped to this reference space. Up to technical details we thus define the effective Hamiltonian as $h := U^\varepsilon\Pi^\varepsilon\widehat{H}\Pi^\varepsilon U^{\varepsilon\,*}$. For the Dirac equation this yields an effective Hamiltonian h_e for electrons acting on the reference space $L^2(\mathbb{R}^3, \mathbb{C}^2)$.
Still h_e is a rather abstract object. However, the effective Hamiltonian allows for an asymptotic expansion in powers of ε, where the leading order terms can be computed explicitly. It turns out that the leading order terms of the effective Hamiltonian yield physically interesting and nontrivial results about the dynamics inside the decoupled subspace.

(iv) **Semiclassical limit.** If the isolated part of the spectrum is an eigenvalue E_* of finite multiplicity, then the effective dynamics in the reference space allows for a simple semiclassical limit. This is because the principal symbol of the effective Hamiltonian is in this case just the eigenvalue $E_*(q, p)$. This fact goes in physics under the name of Peierls' substitution. However, the corrections to Peierls' substitution carry important physical information. In our running example the subprincipal symbol of the effec-

tive electron Hamiltonian h_{e} describes the leading order spin-dynamics. The semiclassical limit for h_{e} yields the T-BMT equation.

Before we proceed with the details, a few remarks on the literature are in order. More detailed references can be found within the specific sections. To our knowledge, the notion "almost invariant subspace" was first coined by Nenciu [Nen$_2$] in the context of gauge invariant perturbation theory. In the context of space-adiabatic problems Brummelhuis and Nourrigat [BrNo] construct Π^ε for the particular case of the Dirac equation and Martinez and Sordoni [MaSo] based on [So] consider Born-Oppenheimer type Hamiltonians. The general scheme for the construction of Π^ε is sketched in Nenciu and Sordoni [NeSo] and applied to the matrix-valued Klein-Gordon equation. Our construction is based on the one in [NeSo], but differs in a few technical details.

Our approach for the construction of the unitary U^ε is specifically designed to deal also with problems as the Dirac equation and the Bloch electron with external magnetic fields, where the projector Π^ε has no limit for $\varepsilon \to 0$, see Remark 3.13. While the specific application is new, the general idea to construct a pseudodifferential operator which is almost unitary and diagonalizes a given pseudodifferential operator has a long tradition, [Ni] Section 7 and references therein, [Ta], [HeSj]. The method of successive diagonalization is also prominent in the physics literature, for example [FoWo] in the derivation of the Pauli equation and its corrections, [Bl$_1$, Bl$_2$] for periodic Schrödinger operators, [Bl$_3$] for the Dirac equation, [LiFl$_1$, LiWe$_1$] for Born-Oppenheimer type Hamiltonians.

After this informal outline we proceed with the details. For the general space-adiabatic theory of the present chapter we assume one of the following conditions.

Condition of increasing gap (IG)$_m$. *Let $H \in S^m_\rho(\varepsilon, \mathcal{L}(\mathcal{H}_{\mathrm{f}}))$ be a hermitian symbol with $\rho > 0$ and $m \geq 0$, such that its principal symbol H_0 satisfies condition (Gap)$_\gamma$ with $\gamma = m$ and assume in addition that $\widehat{H}$ is essentially self-adjoint on $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}})$.*

Condition of constant gap (CG). *Let $H \in S^0_0(\varepsilon, \mathcal{L}(\mathcal{H}_{\mathrm{f}}))$ be a hermitian symbol such that its principal symbol H_0 satisfies condition (Gap)$_\gamma$ with $\gamma = 0$.*

Remark 3.1. The gap condition **(Gap)**$_\gamma$ as a global gap condition is rather strong and also not satisfied in some relevant applications. We saw in Chapter 2 how to obtain local results for the time-dependent Born-Oppenheimer approximation in leading order. We emphasize that also the following constructions are local, and in principle similar techniques as in Chapter 2 could be used to obtain local results. ♢

3.1 Almost invariant subspaces

The content of this section is the *space-adiabatic theorem*. It states that there are subspaces $\Pi^\varepsilon\mathcal{H}$ associated with isolated spectral bands $\sigma_*(z)$ of the principal symbol H_0 of the Hamiltonian $\widehat{H}$ which are approximately invariant under the time-evolution.

Constructions similar to the one presented here appeared several times in the literature. Brummelhuis and Nourrigat [BrNo] gave a proof for the Dirac equation, Martinez and Sordoni [MaSo] considered Born-Oppenheimer type Hamiltonians (cf. Section 4.2) based on results from [So], and Nenciu and Sordoni [NeSo] sketched the general scheme and applied it to a matrix-valued Klein-Gordon type problem.

From now on we denote the spectral projector of $H_0(z)$ corresponding to $\sigma_*(z)$ by $\pi_0(z)$. This change of notation compared to the previous chapters is necessary, since now $\pi_0(z)$ is the principal symbol of the projection on the the approximately invariant subspace we shall construct. The notation $\mathcal{O}_0(\varepsilon^\infty)$ is defined in (A.16), but we recall for the convenience of the reader that $A \in \mathcal{L}(\mathcal{H})$ is $\mathcal{O}_0(\varepsilon^\infty)$ if for all $n \in \mathbb{N}$ there exists a constant $C_n < \infty$ such that $\|A\|_{\mathcal{L}(\mathcal{H})} \leq C_n\varepsilon^n$.

Theorem 3.2 (Space-adiabatic theorem).
Assume either $\mathbf{(IG)}_m$ *or* **(CG)**. *Let* $\widehat{H}$ *be the Weyl quantization of* H. *Then there exists an orthogonal projection* $\Pi^\varepsilon \in \mathcal{L}(\mathcal{H})$ *such that*

$$\left[\,\widehat{H},\,\Pi^\varepsilon\,\right] = \mathcal{O}_0(\varepsilon^\infty) \tag{3.1}$$

and $\Pi^\varepsilon = \widehat{\pi} + \mathcal{O}_0(\varepsilon^\infty)$, *where* $\widehat{\pi}$ *is the Weyl quantization of a semiclassical symbol*

$$\pi \asymp \sum_{j\geq 0} \varepsilon^j \pi_j \qquad \text{in} \quad S^0_\rho(\varepsilon)\,.$$

The principal symbol $\pi_0(z)$ *is the spectral projection of* $H_0(z)$ *corresponding to* $\sigma_*(z)$.

As an immediate consequence of Theorem 3.2, the subspace $\Pi^\varepsilon\mathcal{H}$ is an approximately invariant subspace for the dynamics generated by the Hamiltonian $\widehat{H}$.

Corollary 3.3. *Under the same assumptions as in Theorem 3.2 we have that*

$$\left[\,\mathrm{e}^{-\mathrm{i}\widehat{H}s},\,\Pi^\varepsilon\,\right] = \mathcal{O}_0(\varepsilon^\infty|s|)\,.$$

Proof. Although this is straightforward, we explicitly write out the computation, since the result is of central importance to us.

$$\begin{aligned}\left\| \left[\mathrm{e}^{-\mathrm{i}\widehat{H}s}, \, \Pi^\varepsilon \right] \right\|_{\mathcal{L}(\mathcal{H})} &= \left\| \int_0^s \mathrm{d}s' \, \frac{\mathrm{d}}{\mathrm{d}s'} \left(\mathrm{e}^{\mathrm{i}\widehat{H}s'} \, \Pi^\varepsilon \, \mathrm{e}^{-\mathrm{i}\widehat{H}s'} \right) \right\|_{\mathcal{L}(\mathcal{H})} \\ &= \left\| \int_0^s \mathrm{d}s' \, \mathrm{e}^{\mathrm{i}\widehat{H}s'} \left[\, \widehat{H}, \, \Pi^\varepsilon \, \right] \mathrm{e}^{-\mathrm{i}\widehat{H}s'} \right\|_{\mathcal{L}(\mathcal{H})} \\ &\leq |s| \left\| \left[\, \widehat{H}, \, \Pi^\varepsilon \, \right] \right\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon^\infty \, |s|) \, . \end{aligned}$$

□

We emphasize once more that the subspace $\Pi^\varepsilon \mathcal{H}$ is in general *not* spectral, but it is associated with the spectral band $\sigma_*(z)$.

Remark 3.4. In order to avoid misunderstandings we remind the reader that all operators which arise as Weyl-quantizations of symbols depending on p are ε-dependent. This ε-dependence stems from the quantization rule $p \mapsto -\mathrm{i}\varepsilon\nabla_x$ and possibly also from an explicit dependence of the symbol on ε. In particular the Hamiltonian $\widehat{H}$ is an ε-dependent operator. In order to not overburden notation, we dropped the index ε for such operators, but keep in mind that in most cases the $\widehat{\ }$ implies also an ε-dependence. ♢

Remark 3.5. The terminology "almost invariant subspace" for $\Pi^\varepsilon \mathcal{H}$ is borrowed from [Nen$_2$], although $\Pi^\varepsilon \mathcal{H}$ is, in general, *not* an almost invariant subspace in the sense of [Nen$_2$], since Π^ε need not have a limit as $\varepsilon \to 0$. ♢

Remark 3.6. Notice another consequence of Corollary 3.3, which was anticipated in Section 1.2.2. Since $\|\Pi^\varepsilon - \widehat{\pi}_0\| = \mathcal{O}(\varepsilon)$, it follows that

$$\left[\, \mathrm{e}^{-\mathrm{i}\widehat{H}s}, \, \widehat{\pi}_0 \, \right] = \mathcal{O}_0(\varepsilon + \varepsilon^\infty |s|) \, .$$

This improves the results of Chapter 2, cf. e.g. (2.20), since it shows that solutions of the Schrödinger equation approximately remain in the unperturbed subspaces for times much longer than expected from the analysis of Chapter 2. ♢

Remark 3.7. Note that the growth condition on the gap in $\mathbf{(IG)}_m$ is stronger than one would expect from the analysis in Chapters 2 and 6 or in [NeSo]. Indeed, in both examples a gap which is bounded globally over phase space suffices to prove uniform adiabatic decoupling also in the presence of a Hamiltonian with principal symbol increasing linearly in momentum. More general uniform adiabatic decoupling should hold whenever $\mathbf{(IG)}_m$ is satisfied with $\gamma = m - \rho$. Indeed (3.1) follows from the following proof with slight modifications under this weaker condition on the growth of the gap. However, this modified proof does not give $\pi \in S^0_\rho(\varepsilon)$, a fact we will make use of in the following sections. To avoid further complications in the presentation, we decided to state only the stronger result for the stronger growth condition. ♢

Proof (of Theorem 3.2). We decompose the proof into two steps. First the symbol π of the Moyal projector is constructed and then its quantization $\widehat{\pi}$ is modified in order to obtain a true projector Π^{ε}.

Step I. Construction of the Moyal projector

In general π_0 is not a projector in the Moyal algebra, i.e.

$$\pi_0 \sharp \pi_0 \neq \pi_0 \,.$$

The following lemma shows that π_0 can be corrected, order by order in ε, so to obtain a true Moyal projector π which Moyal commutes with H. Similar constructions appeared in the context of the Schrödinger equation several times in the literature [HeSj, NeSo, BrNo, EmWe]. Our proof was strongly influenced by the one in [NeSo], but differs in relevant details, since we consider different symbol classes. It relies on the construction of the *local* Moyal resolvent of $H_0(z)$. The construction of the global inverse of an elliptic symbol, often called the parametrix, is well known [DiSj, Fo, Ni, Ma$_1$].

Lemma 3.8. *Assume either* $\mathbf{(IG)}_m$ *or* **(CG)**. *Then there exists a* unique *formal symbol*

$$\pi = \sum_{j\geq 0} \varepsilon^j \pi_j \qquad \pi_j \in S^{-j\rho}_{\rho}(\mathcal{L}(\mathcal{H}_{\mathrm{f}}))\,,$$

such that $\pi_0(z)$ *is the spectral projection of* $H_0(z)$ *corresponding to* $\sigma_*(z)$, *with the following properties:*

(i) $\pi \sharp \pi = \pi$,
(ii) $\pi^* = \pi$,
(iii) $H \sharp \pi - \pi \sharp H = 0$.

Proof. We give the proof under the assumption $\mathbf{(IG)}_m$. The proof under assumption **(CG)** is simpler, since all the symbols which appear belong to $S^0_0(\varepsilon)$.

We first provide a constructive scheme for the special case where $\sigma_*(z) = \{E_*(z)\}$ is an eigenvalue, which, at the same time, proves uniqueness of π in the general case. Doing so we follow in principle the construction as given in [EmWe], differ, however, in the presentation. The reason for including this scheme is that the aim of adiabatic perturbation theory is, in particular, to give an as simple as possible recipe for explicitly computing the relevant quantities. The inductive scheme for constructing π in the special case $\sigma_*(z) = \{E_*(z)\}$ is much better suited for explicit computations than the general construction which will follow later on.

Note that

$$\pi_0 \sharp \pi_0 - \pi_0 = \pi_0 \,\pi_0 - \pi_0 + \mathcal{O}(\varepsilon) = \mathcal{O}(\varepsilon)$$

and

$$[H_0, \pi_0]_\sharp = [H_0, \pi_0] + \mathcal{O}(\varepsilon) = \mathcal{O}(\varepsilon)\,.$$

We proceed by induction and assume that we found $\pi^{(n)} = \sum_{j=0}^{n} \varepsilon^j \pi_j$ such that

$$\pi^{(n)} \sharp \pi^{(n)} - \pi^{(n)} = \varepsilon^{n+1}\, G_{n+1} + \mathcal{O}(\varepsilon^{n+2})\,, \tag{3.2}$$

where (3.2) defines G_{n+1}. Thus the next order term in the expansion π_{n+1} must satisfy

$$\pi_{n+1}\,\pi_0 + \pi_0\,\pi_{n+1} - \pi_{n+1} = -G_{n+1}\,, \tag{3.3}$$

which uniquely determines the diagonal part of π_{n+1} to be

$$\pi_{n+1}^{\mathrm{D}} = -\pi_0\, G_{n+1}\,\pi_0 + (1-\pi_0)\, G_{n+1}\,(1-\pi_0)\,. \tag{3.4}$$

Here and in the following we define the diagonal resp. off-diagonal part of an operator A with respect to some orthogonal projection P as

$$A^{\mathrm{D}} = P\,A\,P + (\mathbf{1}-P)\,A\,(\mathbf{1}-P)\,, \quad A^{\mathrm{OD}} = A - A^{\mathrm{D}}\,.$$

Equation (3.3) puts no constraint on the off-diagonal part of π_{n+1}. In particular, $\omega^{(n)} := \pi^{(n)} + \varepsilon^{n+1}\pi_{n+1}^{\mathrm{D}}$ satisfies (i) up to an error of order $\mathcal{O}(\varepsilon^{n+2})$ if and only if

$$G_{n+1} = \pi_0\, G_{n+1}\,\pi_0 + (\mathbf{1}-\pi_0)\, G_{n+1}\,(\mathbf{1}-\pi_0)\,,$$

i.e. $G_{n+1}^{\mathrm{OD}} = 0$. This, however, follows from the fact that G_{n+1} is the principal symbol of $\varepsilon^{-n-1}(\pi^{(n)} \sharp \pi^{(n)} - \pi^{(n)})$. Using (3.2) one finds, e.g.,

$$\begin{aligned}
\pi_0\, G_{n+1}\,(\mathbf{1}-\pi_0) &= \big(\varepsilon^{-n-1}\,\pi_0(\pi^{(n)} \sharp \pi^{(n)} - \pi^{(n)})(\mathbf{1}-\pi_0)\big)_0 \\
&= \big(\varepsilon^{-n-1}\,\pi^{(n)} \sharp (\pi^{(n)} \sharp \pi^{(n)} - \pi^{(n)}) \sharp (\mathbf{1}-\pi^{(n)})\big)_0 \\
&= -\big((\pi^{(n)} \sharp \pi^{(n)} - \pi^{(n)})\, G_{n+1}\big)_0 = 0\,.
\end{aligned}$$

As induction assumption we also have that

$$[H, \pi^{(n)}]_\sharp = \mathcal{O}(\varepsilon^{n+1})$$

and thus

$$[H, \omega^{(n)}]_\sharp = \varepsilon^{n+1} F_{n+1} + \mathcal{O}(\varepsilon^{n+2})\,. \tag{3.5}$$

The diagonal part of π_{n+1} being fixed already, the off-diagonal part π_{n+1}^{OD} must satisfy $[H_0, \pi_{n+1}^{\mathrm{OD}}] = -F_{n+1}$. In particular,

$$\begin{aligned}
H_0(z)\;(\pi_0(z)\pi_{n+1}(z)(1-\pi_0(z))) - (\pi_0(z)\pi_{n+1}(z)(1-\pi_0(z)))\;H_0(z) \\
= -\,\pi_0(z)\,F_{n+1}(z)\,(1-\pi_0(z))
\end{aligned} \tag{3.6}$$

for all $z \in \mathbb{R}^{2d}$.

We first show that if (3.6) has a solution

$$\pi_{n+1}^{OD1}(z) := \pi_0(z)\pi_{n+1}(z)(1-\pi_0(z))\,,$$

then it is unique, i.e. that the kernel of the map $\pi_{n+1}^{OD1}(z) \mapsto [H_0(z), \pi_{n+1}^{OD1}(z)]$ restricted to $(1-\pi_0(z))\mathcal{H}_{\rm f}$ contains only zero. To see this let

$$\widetilde{\sigma}_*(z) := (\sup \sigma_*(z) - \inf \sigma_*(z))/2$$

and note that, due to the gap condition, $H_0(z) - \widetilde{\sigma}_*(z)$ is invertible on $(1-\pi_0(z))\mathcal{H}$ with

$$\|(H_0(z) - \widetilde{\sigma}_*(z))^{-1}(1-\pi_0(z))\| < 2/\mathrm{diam}(\sigma_*(z))\,. \tag{3.7}$$

Hence

$$\begin{aligned}
&[H_0(z), \pi_{n+1}^{OD1}(z)] = 0 \\
&\quad \Leftrightarrow [H_0(z) - \widetilde{\sigma}_*(z), \pi_{n+1}^{OD1}(z)] = 0 \\
&\quad \Leftrightarrow \pi_{n+1}^{OD1}(z) = (H_0(z) - \widetilde{\sigma}_*(z))\pi_{n+1}^{OD1}(z)(H_0(z) - \widetilde{\sigma}_*(z))^{-1}
\end{aligned}$$

and therefore

$$\begin{aligned}
&\|\pi_{n+1}^{OD1}(z)\| \leq \\
&\leq \|(H_0(z) - \widetilde{\sigma}_*(z))\pi_0(z)\|\, \|\pi_{n+1}^{OD1}(z)\|\, \|(H_0(z) - \widetilde{\sigma}_*(z))^{-1}(1-\pi_0(z))\| \\
&= C\, \|\pi_{n+1}^{OD1}(z)\|\,.
\end{aligned}$$

However, from $\|(H_0(z) - \widetilde{\sigma}_*(z))\pi_0(z)\| \leq \mathrm{diam}(\sigma_*(z))/2$ and (3.7) it follows that $C < 1$ and thus $\pi_{n+1}^{OD1}(z) = 0$. We conclude that π_{n+1} is unique when it exists.

In the special case that $\sigma_*(z) = \{E_*(z)\}$, (3.6) can be solved, and one finds

$$\pi_0 \pi_{n+1}(1-\pi_0) = \pi_0\, F_{n+1}\, (H_0 - E_*)^{-1}\, (1-\pi_0)\,. \tag{3.8}$$

Using that F_{n+1} is the principal symbol of $\varepsilon^{-n-1}[H, \omega^{(n)}]_\sharp$, that π_0 is the principal symbol of $\omega^{(n)}$ and that $\omega^{(n)}$ satisfies (i) up to $\mathcal{O}(\varepsilon^{n+2})$, one finds that $\pi_0 F_{n+1} \pi_0 = (1-\pi_0)F_{n+1}(1-\pi_0) = 0$ and thus that $\pi^{(n+1)}$ defined through (3.4) and (3.8) satisfies (i) and (iii) up to $\mathcal{O}(\varepsilon^{n+2})$.

Remark 3.9. For later reference we emphasize that we obtained an explicit, inductive construction for π when $\sigma_*(z) = \{E_*(z)\}$. The latter one involves four steps at each order:

(a) Evaluation of G_{n+1} as in (3.2).
(b) Computation of $\pi_{n+1}^{\rm D}$ as in (3.4).
(c) Evaluation of F_{n+1} as in (3.5).
(d) Computation of $\pi_{n+1}^{\rm OD}$ as in (3.8). ♢

We now turn to the construction of π in the general case. Since the Moyal product is a local operation (it depends only on the pointwise value of the symbols and their derivatives) it suffices to construct π locally in phase space and then uniqueness will liberate us from gluing the local results together.

Let us fix a point $z_0 \in \mathbb{R}^{2d}$. From the continuity of the map $z \mapsto H_0(z)$ and the gap condition it follows that there exists a neighborhood $\mathcal{U}_{z_0}$ of z_0 such that for every $z \in \mathcal{U}_{z_0}$ the set $\sigma_*(z)$ can be enclosed in a positively-oriented complex circle $\Gamma(z_0)$ independent of z in such a way that $\Gamma(z_0)$ is symmetric with respect to the real axis,

$$\operatorname{dist}(\Gamma(z_0), \sigma(z)) \geq \frac{1}{4} C_{\mathrm{g}} \langle p \rangle^{\gamma} \quad \text{for all} \quad z \in \mathcal{U}_{z_0} \tag{3.9}$$

and

$$\operatorname{Radius}(\Gamma(z_0)) \leq C_{\mathrm{r}} \langle p \rangle^{\gamma} \quad \text{for all} \quad z \in \mathcal{U}_{z_0} \tag{3.10}$$

where $\operatorname{Radius}(\Gamma(z_0))$ is the radius of the complex circle $\Gamma = \Gamma(z_0)$. The constant C_{g} in (3.9) is the same as in (G2) and the existence of a constant C_{r} *independent* of z_0 such that (3.10) is satisfied follows from assumption (G3). We keep γ in the notation as a bookkeeping device, in order to distinguish the contributions related to the gap, although $\gamma = m$.

Let us choose any $\zeta \in \Gamma$ and restrict all the following expressions to $z \in \mathcal{U}_{z_0}$. There exist a formal symbol $R(\zeta)$ – the *local Moyal resolvent* of H – such that

$$R(\zeta) \sharp (H - \zeta) = \mathbf{1} = (H - \zeta) \sharp R(\zeta) \qquad \text{on } \mathcal{U}_{z_0}\,. \tag{3.11}$$

The symbol $R(\zeta)$ can be explicitly constructed. We abbreviate

$$R_0(\zeta) = (H_0 - \zeta)^{-1}$$

where the inverse is understood in the $\mathcal{L}(\mathcal{H}_{\mathrm{f}})$-sense and exists according to (3.9). Note that

$$R_0(\zeta) \sharp (H - \zeta) = \mathbf{1} + \mathcal{O}(\varepsilon)\,.$$

We proceed by induction and suppose that

$$R^{(n)}(\zeta) = \sum_{j=0}^{n} \varepsilon^j R_j(\zeta)$$

satisfies the first equality in (3.11) up to $\mathcal{O}(\varepsilon^{n+1})$, i.e.

$$R^{(n)}(\zeta) \sharp (H - \zeta) = \mathbf{1} + \varepsilon^{n+1} E_{n+1}(\zeta) + \mathcal{O}(\varepsilon^{n+2})\,.$$

By choosing

$$R_{n+1}(\zeta) = -E_{n+1}(\zeta)\,(H_0 - \zeta)^{-1}\,,$$

we obtain that $R^{(n+1)}(\zeta) = R^{(n)}(\zeta) + \varepsilon^{n+1} R_{n+1}(\zeta)$ satisfies the same equality up to $\mathcal{O}(\varepsilon^{n+2})$. Then the formal symbol $R(\zeta) = \sum_{j \geq 0} \varepsilon^j R_j(\zeta)$ satisfies the first equality in (3.11) which – by the associativity of the Moyal product – implies the second one. More precisely, denote the symbol just constructed as $R_{\mathrm{l}}(\zeta)$, the left resolvent. An analogous construction yields $R_{\mathrm{r}}(\zeta)$, the right

resolvent, which satisfies $\mathbf{1} = (H - \zeta) \sharp R_{\mathrm{r}}(\zeta)$. Multiplying this identity with $R_{\mathrm{l}}(\zeta)$ from the left and using associativity of the Moyal product, one obtains

$$R_{\mathrm{l}}(\zeta) = R_{\mathrm{l}}(\zeta) \sharp \big((H - \zeta) \sharp R_{\mathrm{r}}(\zeta)\big) = \big(R_{\mathrm{l}}(\zeta) \sharp (H - \zeta)\big) \sharp R_{\mathrm{r}}(\zeta) = R_{\mathrm{r}}(\zeta)\,.$$

Observe that (3.11) implies, as in the case of operators, that $R(\zeta)$ satisfies the resolvent equation

$$R(\zeta) - R(\zeta') = (\zeta - \zeta')\, R(\zeta) \sharp R(\zeta') \qquad \text{on } \mathcal{U}_{z_0}\,. \tag{3.12}$$

From the resolvent equation it follows – by using an argument similar to the standard one in operator theory [Ka$_1$] – that the symbol $\pi = \sum_{j\geq 0} \varepsilon^j \pi_j$ defined by

$$\pi_j(z) = \frac{\mathrm{i}}{2\pi} \oint_{\Gamma} \mathrm{d}\zeta\, R_j(\zeta, z)\,, \qquad z \in \mathcal{U}_{z_0}\,, \tag{3.13}$$

is a Moyal projector such that $[H, \pi]_\sharp = 0$ on $\mathcal{U}_{z_0}$. Indeed, for every fixed $z \in \mathcal{U}_{z_0}$ and $j \in \mathbb{N}$, the map $\zeta \mapsto R_j(\zeta, z)$ is holomorphic in a neighborhood of the circle $\Gamma(z_0)$. Then $\Gamma(z_0)$ can be expanded to a slightly larger circle Γ' without changing the left hand side of (3.13) and we obtain

$$\begin{aligned}
(\pi \sharp \pi)_j &= \left(\frac{\mathrm{i}}{2\pi}\right)^2 \oint_{\Gamma'} \mathrm{d}\zeta' \oint_{\Gamma} \mathrm{d}\zeta \left(R(\zeta') \sharp R(\zeta)\right)_j \\
&= \left(\frac{\mathrm{i}}{2\pi}\right)^2 \oint_{\Gamma'} \mathrm{d}\zeta' \oint_{\Gamma} \mathrm{d}\zeta\, (\zeta' - \zeta)^{-1} \left(R(\zeta') - R(\zeta)\right)_j \\
&= \frac{\mathrm{i}}{2\pi} \oint_{\Gamma} \mathrm{d}\zeta\, R_j(\zeta) = \pi_j\,,
\end{aligned} \tag{3.14}$$

where (3.12) has been used. The first equality in (3.14) follows by noticing that for every $\alpha \in \mathbb{N}^{2d}$

$$\partial_z^\alpha \pi_j(z) = \frac{\mathrm{i}}{2\pi} \oint_{\Gamma} \mathrm{d}\zeta\, \partial_z^\alpha R_j(\zeta, z) \qquad z \in \mathcal{U}_{z_0}\,,$$

and by expanding the Moyal product order by order in ε.

Since the circle Γ is symmetric with respect to the real axis one immediately concludes that $\pi^* = \pi$, since $R(\zeta)^* = R(\bar{\zeta})$ as a consequence of (3.11). Recall that according to (3.13) we have that

$$\pi = \frac{\mathrm{i}}{2\pi} \oint_{\Gamma} \mathrm{d}\zeta\, R(\zeta)$$

on $\mathcal{U}_{z_0}$ and from the resolvent equation is follows that $[R(\zeta), R(\zeta')]_\sharp = 0$ for all $\zeta, \zeta' \in \Gamma$. Hence π Moyal-commutes with $R(\zeta')$ for any $\zeta' \in \Gamma$. Then, by multiplying $\pi \sharp R(\zeta') = R(\zeta') \sharp \pi$ by $(H - \zeta')$ on both sides, one obtains that $H \sharp \pi = \pi \sharp H$.

Up to now we remained purely on a formal series level. In order to obtain useful results after quantization, one needs to control the growth of the symbols. For the Lemma we have to show that $\pi_j \in S^{-j\rho}_{\rho}$ for every $j \in \mathbb{N}$. From the Riesz formula (3.13) it follows that for every $\alpha \in \mathbb{N}^{2d}$ one has

$$\left\|\left(\partial_z^\alpha \pi_j\right)(z)\right\|_{\mathcal{L}(\mathcal{H}_{\rm f})} \leq \mathrm{Radius}\left(\Gamma(z_0)\right) \sup_{\zeta\in\Gamma(z_0)} \left\|\left(\partial_z^\alpha R_j\right)(\zeta,z)\right\|_{\mathcal{L}(\mathcal{H}_{\rm f})} .$$

According to (3.10) we are left to prove that

$$\sup_{\zeta\in\Gamma(z_0)} \left\|\left(\partial_q^\alpha \partial_p^\beta R_j\right)(\zeta,z)\right\|_{\mathcal{L}(\mathcal{H}_{\rm f})} \leq C_{\alpha\beta j} \left\langle p\right\rangle^{-\gamma-j\rho-|\beta|\rho} , \quad \alpha,\beta \in \mathbb{N}^d,\ j\in\mathbb{N}, \tag{3.15}$$

where $C_{\alpha\beta j}$ must *not* depend on z_0. As for R_0, we notice that according to (3.9) one has

$$\left\|\left(H_0(z)-\zeta\right)^{-1}\right\|_{\mathcal{L}(\mathcal{H}_{\rm f})} \leq \frac{1}{\mathrm{dist}(\zeta,\sigma(H_0(z)))} \leq \frac{4}{C_{\rm g}} \left\langle p\right\rangle^{-\gamma} , \tag{3.16}$$

and moreover,

$$\begin{aligned} \left\|\nabla_p R_0(z)\right\|_{\mathcal{L}(\mathcal{H}_{\rm f})} &= \left\|(R_0 \nabla_p H_0 R_0)(z)\right\|_{\mathcal{L}(\mathcal{H}_{\rm f})} \\ &\leq \left(\frac{4}{C_{\rm g}}\right)^2 \left\langle p\right\rangle^{-2\gamma} \left\|\nabla_p H_0(z)\right\|_{\mathcal{L}(\mathcal{H}_{\rm f})} \\ &\leq C \left\langle p\right\rangle^{-2\gamma+m-\rho} = C\left\langle p\right\rangle^{-\gamma-\rho} , \end{aligned}$$

where the last bound follows from the fact that $H_0 \in S^m_\rho$ (recall that $\gamma = m$). By induction one controls higher order derivatives and (3.15) follows for $j = 0$.

Again by induction, assume that $R_0, \ldots, R_n$ satisfy the bound (3.15). Then, by writing out

$$E_{n+1} = \Big(R^{(n)}(\zeta) \sharp (H-\zeta) - 1\Big)_{n+1}$$

and using (A.9), one concludes that $R_{n+1} = -E_{n+1}R_0$ satisfies (3.15) with $\gamma = m$. □

Step II. Quantization

First of all, by resummation, cf. Proposition A.14, we obtain a semiclassical symbol $\pi : \mathbb{R}^{2d} \times [0,\varepsilon_0) \to \mathcal{L}(\mathcal{H}_{\rm f})$ whose asymptotic expansion is given by $\sum_{j\geq 0} \varepsilon^j \pi_j$. Then, by Weyl quantization, one gets a bounded operator $\widehat{\pi} \in \mathcal{L}(\mathcal{H}_{\rm f})$, see Proposition A.6, which is an almost-projector, in the sense that

(i) $\widehat{\pi}^2 = \widehat{\pi} + \mathcal{O}_{-\infty}(\varepsilon^\infty)$,
(ii) $\widehat{\pi}^* = \widehat{\pi}$,
(iii) $[\,\widehat{H}, \widehat{\pi}\,] = \mathcal{O}_{-\infty}(\varepsilon^\infty)$.

Remark 3.10. Notice that the assumption $\rho > 0$ is crucial in order to obtain (iii) for an unbounded $\widehat{H}$, i.e. for $H \in S^m_\rho$ with $m > 0$. For $\rho = 0$ we could, in general, only conclude that $[H, \pi]_\sharp = \mathcal{O}(\varepsilon^\infty)$ in S^m_0, which does not imply that the commutator of the operators is small in the norm of bounded operators. $\diamondsuit$

In order to turn $\widehat{\pi}$ into a true projector which is $\mathcal{O}(\varepsilon)$-close to $\widehat{\pi}$, we follow an idea from [NeSo]. Notice that $\|\widehat{\pi}^2 - \widehat{\pi}\| = \mathcal{O}(\varepsilon^\infty)$ and hence the spectral mapping theorem for self-adjoint operators implies that for each $n \in \mathbb{N}$ there is a $C_n < \infty$ such that

$$\sigma(\widehat{\pi}) \subset [-C_n\varepsilon^n, C_n\varepsilon^n] \cup [1 - C_n\varepsilon^n, 1 + C_n\varepsilon^n] =: \sigma_0^\varepsilon \cup \sigma_1^\varepsilon \,.$$

For $\varepsilon \leq 1/(4C_1)$ one can thus define

$$\Pi^\varepsilon = \frac{\mathrm{i}}{2\pi} \oint_{|\zeta-1|=\frac{1}{2}} \mathrm{d}\zeta \, (\widehat{\pi} - \zeta)^{-1} \,.$$

Then $\Pi^{\varepsilon\,2} = \Pi^\varepsilon$ follows and we claim that $\Pi^\varepsilon = \widehat{\pi} + \mathcal{O}_0(\varepsilon^\infty)$. Indeed,

$$\widehat{\pi} = \int_{\sigma_0^\varepsilon \cup \sigma_1^\varepsilon} \lambda E(\mathrm{d}\lambda) = \mathcal{O}_0(\varepsilon^n) + \int_{\sigma_1^\varepsilon} E(\mathrm{d}\lambda) = \Pi^\varepsilon + \mathcal{O}_0(\varepsilon^n) \qquad \text{for all } n \in \mathbb{N} \,,$$

where $E(\cdot)$ is the projection valued measure of $\widehat{\pi}$. Finally notice that

$$\begin{aligned} [\widehat{H}, \Pi^\varepsilon] &= \frac{\mathrm{i}}{2\pi} \oint_{|\zeta-1|=\frac{1}{2}} \mathrm{d}\zeta \, [\widehat{H}, (\widehat{\pi} - \zeta)^{-1}] \\ &= -\frac{\mathrm{i}}{2\pi} \oint_{|\zeta-1|=\frac{1}{2}} \mathrm{d}\zeta \, (\widehat{\pi} - \zeta)^{-1} [\widehat{H}, \widehat{\pi}] (\widehat{\pi} - \zeta)^{-1} \,, \end{aligned}$$

which implies that

$$\big\| [\widehat{H}, \Pi^\varepsilon] \big\|_{\mathcal{L}(\mathcal{H})} \leq C \big\| [\widehat{H}, \widehat{\pi}] \big\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}_0(\varepsilon^\infty) \,.$$

This concludes the proof of the theorem. □

3.2 Mapping to the reference space

The fact that the subspace associated with an isolated energy band decouples from its orthogonal complement up to small errors in ε leads immediately to the following question. Is there a natural way to describe the dynamics of the system inside the almost invariant subspace $\Pi^\varepsilon\mathcal{H}$? The main obstruction for such a simple description is the fact that the subspace $\Pi^\varepsilon\mathcal{H}$ depends on ε and cannot be easily characterized. Even worse, in general the limit $\lim_{\varepsilon\to 0} \Pi^\varepsilon$ does not exist, meaning that $\Pi^\varepsilon\mathcal{H}$ is not even close to an ε-independent

subspace. In order to obtain a useful description of the effective intraband dynamics we thus need to map $\Pi^\varepsilon\mathcal{H}$ to an easily accessible and ε-independent reference subspace. As a simple example recall the map $\mathcal{U} : P_*\mathcal{H} \to L^2(\mathbb{R}^{3l})$ from the Born-Oppenheimer setting defined in (1.44), which maps the wave functions in the band subspace $P_*\mathcal{H}$ to a wave function for the nuclei only. In general this "mapping to the reference space" is not so simple anymore, as we shall see in the following.

The choice of the reference space is canonical even in the general setting. This is because the smoothness of $(q,p) \mapsto H_0(q,p)$ and the gap condition imply by the same argument as in Section 2.1 that the map $(q,p) \mapsto \pi_0(q,p)$ is smooth. Hence there is a subspace $\mathcal{K}_\mathrm{f} \subset \mathcal{H}_\mathrm{f}$ independent of (q,p) such that the subspaces $\pi_0(q,p)\mathcal{H}_\mathrm{f}$ are all isomorphic to $\mathcal{K}_\mathrm{f}$.

Let π_r be the projection onto $\mathcal{K}_\mathrm{f} \subset \mathcal{H}_\mathrm{f}$, then

$$\Pi_\mathrm{r} := \mathbf{1} \otimes \pi_\mathrm{r} \quad (= \widehat{\pi}_\mathrm{r})$$

will serve as the projector onto the *reference subspace* $\mathcal{K} := \Pi_\mathrm{r}\mathcal{H} \subset \mathcal{H}$. This reference subspace does not depend on ε and is constant with respect to the fibration over $\mathbb{R}^d$ and as such we will use it as a *simple* representation of the almost invariant subspace $\Pi^\varepsilon\mathcal{H}$.

Remark 3.11. It is only for convenience and for simpler notation in the following statements and proofs that we take $\mathcal{K}_\mathrm{f}$ as a subspace of $\mathcal{H}_\mathrm{f}$. In applications it will be completely irrelevant how $\mathcal{K}_\mathrm{f}$ is imbedded in $\mathcal{H}_\mathrm{f}$. As a subspace of $\mathcal{H}_\mathrm{f}$ clearly $\mathcal{K}_\mathrm{f}$ is not unique and a convenient choice must be made in concrete applications. However, apart from the non-uniqueness of this embedding, the reference space is canonical. ♢

Once the reference Hilbert space is fixed, the goal is to unitarily map $\Pi^\varepsilon\mathcal{H}$ to $\mathcal{K}$. To this end we chose a smooth unitary operator valued function $u_0(z)$ which pointwise in phase space intertwines $\pi_0(z)$ and π_r, i.e.

$$u_0(z)\,\pi_0(z)\,u_0(z)^* = \pi_\mathrm{r}\,. \tag{3.17}$$

The existence of such a smooth map follows from an argument sketched in Remark 3.17 at the end of this section. Again $u_0(z)$ is not unique and must be chosen conveniently. In most applications there is a natural choice for $u_0(z)$, which reflects the physics of the problem, as will be explained in detail in the examples of Chapter 4 and 5.

Unfortunately we are not able to prove that it is possible to choose u_0 in $S^0_\rho(\mathcal{L}(\mathcal{H}_\mathrm{f}))$. Indeed, relation (3.17) does not imply any bound at infinity on the derivatives of u_0, as can be seen by multiplying u_0 with a highly oscillating phase. Hence we assume that it is possible to chose u_0 such that $u_0 \in S^0_\rho(\mathcal{L}(\mathcal{H}_\mathrm{f}))$, as it will be the case in the physical examples.

In the following $\mathcal{U}(\mathcal{H}_\mathrm{f})$ stands for the group of unitary operators on $\mathcal{H}_\mathrm{f}$.

Theorem 3.12. *Assume either* $\mathbf{(IG)}_m$ *or* **(CG)** *and that there exists a* $\mathcal{U}(\mathcal{H}_\mathrm{f})$*-valued map* $u_0 \in S^0_\rho(\mathcal{L}(\mathcal{H}_\mathrm{f}))$ *which satisfies (3.17). Then there exist a unitary operator* $U^\varepsilon \in \mathcal{L}(\mathcal{H})$ *such that*

$$U^\varepsilon \, \Pi^\varepsilon \, U^{\varepsilon\,*} = \Pi_\mathrm{r} \tag{3.18}$$

and $U^\varepsilon = \widehat{u} + \mathcal{O}_0(\varepsilon^\infty)$*, where* $u \asymp \sum_{j\geq 0} \varepsilon^j u_j$ *in* $S^0_\rho(\varepsilon)$ *with principal symbol* u_0*.*

Remark 3.13. In [NeSo] the Nagy transformation is used in order to map $\mathrm{Ran}\Pi^\varepsilon$ to the ε-independent subspace $\mathrm{Ran}\widehat{\pi}_0$. This is possible because in their application the symbol π_0 depends only on q and, as a consequence, $\widehat{\pi}_0$ is a projector satisfying $\|\Pi^\varepsilon - \widehat{\pi}_0\| = \mathcal{O}(\varepsilon)$. However, in general π_0 depends on q and p and the mapping to the reference space becomes more subtle. ♢

Remark 3.14. Note that no $\mathcal{O}(\varepsilon^\infty)$ appears in (3.18). The fact U^ε can be constructed such that (3.18) holds exactly will prove useful when we compare the true and the effective dynamics in Section 3.3. ♢

Proof. **Step I. Construction of the Moyal unitaries**

Again u_0 fails to be a Moyal unitary, i.e. $u_0^* \sharp u_0 \neq 1$, and to intertwine π and π_r. However, the following lemma shows that u_0 can be corrected order by order to reach this goal. The idea of constructing a pseudodifferential operator which is almost unitary and diagonalizes a given pseudodifferential operator has a long tradition, cf. [Ni] Section 7 and references therein, and was applied in different settings many times, e.g. [Ta, HeSj]. It was also used in the physics literature in a context closely related to ours, cf. Appendix C.

Lemma 3.15. *Assume either* $\mathbf{(IG)}_m$ *or* **(CG)** *and that there exists a* $\mathcal{U}(\mathcal{H}_\mathrm{f})$*-valued map* $u_0 \in S^0_\rho(\mathcal{L}(\mathcal{H}_\mathrm{f}))$ *which satisfies (3.17), where* π_0 *is the principal symbol of some Moyal projector* $\pi \in M^0_\rho(\varepsilon)$ *(e.g. the one constructed in Lemma 3.8). Then there is a formal symbol* $u = \sum_{j\geq 0} \varepsilon^j u_j$*, with* $u_j \in S^{-j\rho}_\rho(\mathcal{L}(\mathcal{H}_\mathrm{f}))$*, such that*

(i) $u^* \sharp u = 1 \qquad$ *and* $\qquad u \sharp u^* = 1\,,$
(ii) $u \sharp \pi \sharp u^* = \pi_\mathrm{r}\,.$

Remark 3.16. We emphasize that – as opposed to the Moyal projector π appearing in Lemma 3.8 – the Moyal unitary u is highly non-unique even for fixed u_0. As it will follow from the proof, all the possible choices of Moyal unitaries intertwining π and π_r with prescribed principal symbol u_0 are parameterized by the antihermitian Moyal symbols which are diagonal in the π_r-splitting. This freedom clearly corresponds to arbitrary unitary transformations inside $\pi_\mathrm{r}\mathcal{H}_\mathrm{f}$ and $\pi_\mathrm{r}^\perp\mathcal{H}_\mathrm{f}$ ♢

Proof (of Lemma 3.15). Observe that u_0 satisfies (i) and (ii) on the principal symbol level. We proceed by induction and assume that we found $u^{(n)} = \sum_{j=0}^{n} \varepsilon^j u_j$ satisfying (i) and (ii) up to $\mathcal{O}(\varepsilon^{n+1})$. We will construct u_{n+1} such that $u^{(n+1)} = u^{(n)} + \varepsilon^{n+1} u_{n+1}$ satisfies (i) and (ii) up to $\mathcal{O}(\varepsilon^{n+2})$. To this end we write without restriction

$$u_{n+1} =: (a_{n+1} + b_{n+1}) u_0 \,, \tag{3.19}$$

with a_{n+1} hermitian and b_{n+1} anti-hermitian. By induction assumption we have

$$\begin{aligned} u^{(n)} \sharp u^{(n)*} - 1 &= \varepsilon^{n+1} A_{n+1} + \mathcal{O}(\varepsilon^{n+2}) \\ u^{(n)*} \sharp u^{(n)} - 1 &= \varepsilon^{n+1} \tilde{A}_{n+1} + \mathcal{O}(\varepsilon^{n+2}) \,. \end{aligned}$$

Thus u_{n+1} has to solve

$$\begin{aligned} u_0 \, u_{n+1}^* + u_{n+1} \, u_0^* &= -A_{n+1}, \\ u_{n+1}^* \, u_0 + u_0^* \, u_{n+1} &= -\tilde{A}_{n+1} \,. \end{aligned} \tag{3.20}$$

Inserting (3.19) into the first equation in (3.20) we find that $a_{n+1} = -\frac{1}{2} A_{n+1}$, since A_{n+1} is hermitian as it is the principal symbol of $\varepsilon^{-n-1}(u^{(n)} \sharp u^{(n)*} - 1)$. The second equation in (3.20) is then also satisfied, since the compatibility equation $u_0 \, \tilde{A}_{n+1} = A_{n+1} \, u_0$ follows from

$$\frac{1}{\varepsilon^{n+1}} \, u^{(n)} \sharp (u^{(n)*} \sharp u^{(n)} - 1) = \frac{1}{\varepsilon^{n+1}} (u^{(n)} \sharp u^{(n)*} - 1) \sharp u^{(n)}$$

by noticing that $u_0 \, \tilde{A}_{n+1}$ (resp. $A_{n+1} \, u_0$) is the principal symbol of the l.h.s (resp. r.h.s).

Note that (3.20) puts no constraint on b_{n+1} and we are left to determine it using (ii). Let $w^{(n)} = u^{(n)} + \varepsilon^{n+1} a_{n+1} u_0$, then by induction assumption

$$w^{(n)} \sharp \pi \sharp w^{(n)*} - \pi_{\mathrm{r}} = \varepsilon^{n+1} B_{n+1} + \mathcal{O}(\varepsilon^{n+2})$$

and thus

$$u^{(n+1)} \sharp \pi \sharp u^{(n+1)*} - \pi_{\mathrm{r}} = \varepsilon^{n+1} \left(B_{n+1} + [b_{n+1}, \pi_{\mathrm{r}}] \right) + \mathcal{O}(\varepsilon^{n+2}) \,.$$

Hence we need to find an anti-hermitian b_{n+1} satisfying

$$B_{n+1} + [b_{n+1}, \pi_{\mathrm{r}}] = 0 \,. \tag{3.21}$$

A solution to (3.21) is given by

$$b_{n+1} = [\pi_{\mathrm{r}}, B_{n+1}] \,, \tag{3.22}$$

provided that B_{n+1} is hermitian and off-diagonal in the π_{r}-splitting, i.e. $\pi_{\mathrm{r}} \, B_{n+1} \, \pi_{\mathrm{r}}$ and $(1 - \pi_{\mathrm{r}}) \, B_{n+1} \, (1 - \pi_{\mathrm{r}})$ vanish. This follows by noticing that B_{n+1} is the principal symbol of $\varepsilon^{-(n+1)} \left(w^{(n)} \sharp \pi \sharp w^{(n)*} - \pi_{\mathrm{r}} \right)$ and then

$$
\begin{aligned}
(1-\pi_{\mathrm{r}})\, B_{n+1}\, (1-\pi_{\mathrm{r}}) &= \left(\frac{1}{\varepsilon^{n+1}} (1-\pi_{\mathrm{r}}) \left(w^{(n)} \sharp \pi \sharp w^{(n)*} - \pi_{\mathrm{r}} \right) (1-\pi_{\mathrm{r}}) \right)_0 \\
&= \left(\frac{1}{\varepsilon^{n+1}} (1-\pi_{\mathrm{r}}) \left(w^{(n)} \sharp \pi \sharp w^{(n)*} \right) (1-\pi_{\mathrm{r}}) \right)_0 \\
&= \left(\frac{1}{\varepsilon^{n+1}} \left(\varepsilon^{2(n+1)} B_{n+1} \left(w^{(n)} \sharp \pi \sharp w^{(n)*} \right) B_{n+1} + \mathcal{O}(\varepsilon^{n+2}) \right) \right)_0 = 0,
\end{aligned}
$$

where for the second to last equality we inserted

$$
1 - \pi_{\mathrm{r}} = w^{(n)} \sharp (1-\pi) \sharp w^{(n)*} + \varepsilon^{n+1} B_{n+1} + \mathcal{O}(\varepsilon^{n+2})
$$

and used that $w^{(n)}$ solves (i) up to $\mathcal{O}(\varepsilon^{n+2})$ and that π is a Moyal projector. A similar argument shows that $\pi_{\mathrm{r}}\, B_{n+1}\, \pi_{\mathrm{r}}$ vanishes too. Note also that (3.22) fixes only the off-diagonal part of b_{n+1} and one is free to choose the diagonal part of b_{n+1} arbitrarily, which is exactly the non-uniqueness mentioned in Remark 3.16.

It remains to show that the assumption $u_0 \in S^0_\rho$ implies that u_j belongs to $S^{-j\rho}_\rho$. Assume by induction that $u^{(n)} \in M^0_\rho(\varepsilon)$. Then the formula

$$
a_{n+1} = -\frac{1}{2} A_{n+1} = -\frac{1}{2} \left(u^{(n)} \sharp u^{(n)*} - 1 \right)_{n+1}
$$

shows that a_{n+1} belongs to $S^{-(n+1)\rho}_\rho$ as it is the $(n+1)^{\text{th}}$ term of an element of $M^0_\rho(\varepsilon)$. By Proposition A.9, $a_{n+1} u_0 \in S^{-(n+1)\rho}_\rho$ as well. Analogously we have that $B_{n+1} \in S^{-(n+1)\rho}_\rho$ by induction assumption, therefore $b_{n+1} \in S^{-(n+1)\rho}_\rho$ and thus $b_{n+1} u_0 \in S^{-(n+1)\rho}_\rho$, which finally gives $u_{n+1} \in S^{-(n+1)\rho}_\rho$. □

Step II. Quantization

Now let u denote a resummation of the formal power series $u = \sum_{j\geq 0} \varepsilon^j u_j$ in $S^0_\rho(\varepsilon)$. Then, by Weyl quantization, one gets a bounded operator $\widehat{u} \in \mathcal{L}(\mathcal{H})$ such that:

(i) $\widehat{u}^* \widehat{u} = 1 + \mathcal{O}_{-\infty}(\varepsilon^\infty)$ and $\widehat{u}\, \widehat{u}^* = 1 + \mathcal{O}_{-\infty}(\varepsilon^\infty)$
(ii) $\widehat{u}\, \widehat{\pi}\, \widehat{u}^* = \Pi_{\mathrm{r}} + \mathcal{O}_{-\infty}(\varepsilon^\infty)$.

As a first step we modify $\widehat{u}$ by an $\mathcal{O}_0(\varepsilon^\infty)$-term in order to get a true unitary operator $\widetilde{U}^\varepsilon \in \mathcal{U}(\mathcal{H})$, which, in general, does not correspond to the Weyl quantization of any semiclassical symbol.

Notice that $\widehat{u}^* \widehat{u}$ is a self-adjoint positive operator which is $\mathcal{O}_0(\varepsilon^\infty)$-close to the identity operator. Then $(\widehat{u}^* \widehat{u})^{-\frac{1}{2}}$ is well defined and again self-adjoint and $\mathcal{O}_0(\varepsilon^\infty)$-close to the identity operator. As a consequence

$$
\widetilde{U}^\varepsilon = \widehat{u}\, (\widehat{u}^* \widehat{u})^{-\frac{1}{2}}\,, \tag{3.23}
$$

is $\mathcal{O}_0(\varepsilon^\infty)$-close to $\widehat{u}$ and, moreover, unitary. The latter fact follows from

$$\widetilde{U}^{\varepsilon}\,\widetilde{U}^{\varepsilon\,*} = \widehat{u}\,(\widehat{u}^{\,*}\widehat{u})^{-1}\,\widehat{u}^{\,*} = \widehat{u}\,\widehat{u}^{\,-1}\,\widehat{u}^{\,*\,-1}\,\widehat{u}^{\,*} = \mathbf{1}$$

and

$$\widetilde{U}^{\varepsilon\,*}\,\widetilde{U}^{\varepsilon} = (\widehat{u}^{\,*}\widehat{u})^{-\frac{1}{2}}\;\widehat{u}^{\,*}\,\widehat{u}\;(\widehat{u}^{\,*}\widehat{u})^{-\frac{1}{2}} = \mathbf{1}\,.$$

Finally one can modify $\widetilde{U}^{\varepsilon}$ in order to obtain a unitary which exactly intertwines Π^{ε} and Π_{r}. Since $\|\widetilde{U}^{\varepsilon}\,\Pi^{\varepsilon}\,\widetilde{U}^{\varepsilon\,*} - \Pi_{\mathrm{r}}\| < 1$ for ε sufficiently small, the Nagy formula

$$W^{\varepsilon} = \Big(\mathbf{1} - \Big(\widetilde{U}^{\varepsilon}\,\Pi^{\varepsilon}\,\widetilde{U}^{\varepsilon\,*} - \Pi_{\mathrm{r}}\Big)^2\Big)^{-\frac{1}{2}}\Big(\Pi_{\mathrm{r}}\,\widetilde{U}^{\varepsilon}\,\Pi^{\varepsilon}\,\widetilde{U}^{\varepsilon\,*} + (\mathbf{1}-\Pi_{\mathrm{r}})(\mathbf{1}-\widetilde{U}^{\varepsilon}\,\Pi^{\varepsilon}\,\widetilde{U}^{\varepsilon\,*})\Big)$$

defines a unitary operator $W^{\varepsilon} \in \mathcal{U}(\mathcal{H})$ such that $W^{\varepsilon}\,\widetilde{U}^{\varepsilon}\,\Pi^{\varepsilon}\,\widetilde{U}^{\varepsilon\,*}\,W^{\varepsilon\,*} = \Pi_{\mathrm{r}}$ and $W^{\varepsilon} = \mathbf{1} + \mathcal{O}_0(\varepsilon^{\infty})$. Thus by defining $U^{\varepsilon} = W^{\varepsilon}\,\widetilde{U}^{\varepsilon}$ one obtains (3.18), with the desired properties. □

Remark 3.17. We sketch how to prove the existence of a smooth map u_0 satisfying (3.17). Given

$$E = \big\{(z,\psi) \in \mathbb{R}^{2d} \times \mathcal{H}_{\mathrm{f}} : \psi \in \pi_0(z)\mathcal{H}_{\mathrm{f}}\big\}\,,$$

the map $P_E : E \to \mathbb{R}^{2d}, (z,\psi) \mapsto z$ defines a fibration of Hilbert spaces over the base space $\mathbb{R}^{2d}$.

The fibration is locally trivial. Indeed for any $z_0 \in \mathbb{R}^{2d}$ there exists a neighborhood $\mathcal{U}_{z_0}$ such that $\|\pi_0(z) - \pi_0(z_0)\| < 1$ for any $z \in \mathcal{U}_{z_0}$, so that the Nagy formula

$$w(z) = \Big(1 - (\pi_0(z) - \pi_0(z_0))^2\Big)^{-\frac{1}{2}}\Big(\pi_0(z)\pi_0(z_0) + (1-\pi_0(z))(1-\pi_0(z_0))\Big)$$

locally defines a unitary operator $w(z)$ such that $w(z)^*\pi_0(z)w(z) = \pi_0(z_0)$. A local trivialization of the fibration is then explicitly given by

$$\begin{aligned}\Theta : P_E^{-1}(\mathcal{U}_{z_0}) \to \mathcal{U}_{z_0} \times \pi(z_0)\mathcal{H}_{\mathrm{f}} \to \quad & \mathcal{U}_{z_0} \times \mathcal{K}_{\mathrm{f}} \\ (z,\psi) \quad \mapsto \quad (z, w(z)\psi) \quad & \mapsto (z, \phi(z_0)w(z)\psi)\end{aligned}$$

where we use the fact that there exists a unitary operator $\phi(z_0) : \pi(z_0)\mathcal{H}_{\mathrm{f}} \to \mathcal{K}_{\mathrm{f}}$. The existence of $\phi(z_0)$ follows from the fact that the dimension of $\pi(z_0)\mathcal{H}_{\mathrm{f}}$ is independent of z_0, but the map $z_0 \mapsto \phi(z_0)$ may be a priori even discontinuous.

Moreover one can check that any two such trivializations are $\mathcal{U}(\mathcal{K}_{\mathrm{f}})$-compatible, and the previous data define a linear $\mathcal{U}(\mathcal{K}_{\mathrm{f}})$-bundle.

Since the base space is contractible, the bundle is trivial and the associated principal $\mathcal{U}(\mathcal{K}_{\mathrm{f}})$-bundle (i.e. the bundle of the orthonormal frames) admits a global smooth section. This implies the existence of a smooth map $u_0 : \mathbb{R}^{2d} \to \mathcal{U}(\mathcal{H}_{\mathrm{f}})$ such that (3.17) holds true. ♢

3.3 Effective dynamics

We are now in a position to determine the effective dynamics on the reference subspace. In the previous section we constructed a unitary U^ε on $\mathcal{H}$ which exactly intertwines the almost invariant subspace $\Pi^\varepsilon\mathcal{H}$ and the reference subspace $\mathcal{K} = \Pi_{\mathrm{r}}\mathcal{H}$. U^ε and Π^ε are $\mathcal{O}_0(\varepsilon^\infty)$-close to pseudodifferential operators with symbols u and π both in $S^0_\rho(\varepsilon)$. As the final step to an effective description of the dynamics inside the adiabatically decoupled subspace one also unitarily rotates the diagonal part

$$H_{\mathrm{diag}} = \Pi^\varepsilon \widehat{H} \Pi^\varepsilon + \Pi^{\varepsilon\,\perp} \widehat{H} \Pi^{\varepsilon\,\perp} = \widehat{H} + \mathcal{O}_0(\varepsilon^\infty)$$

of the Hamiltonian to the reference space.

Definition 3.18. *Let h be a resummation in $S^m_\rho(\varepsilon)$ of the formal symbol*

$$h = u \sharp H \sharp u^* \,. \tag{3.24}$$

Then $\widehat{h}$ is called the effective Hamiltonian on the reference space.

The existence of a resummation of h in $S^m_\rho(\varepsilon)$ follows from $u \in S^0_\rho(\varepsilon)$ and $H \in S^m_\rho(\varepsilon)$ and the product rule, Proposition A.15.

Remark 3.19. It might seem more natural to define the effective Hamiltonian as the rotation of the diagonal part of original Hamiltonian projected onto the almost invariant subspace, i.e. as

$$H' = U^\varepsilon \, H_{\mathrm{diag}} \, U^{\varepsilon\,*} \,. \tag{3.25}$$

Clearly one should have $H' - \widehat{h} = \mathcal{O}(\varepsilon^\infty)$ in some sense. However, if $\widehat{H}$ is unbounded, this closeness does not follow in the norm of bounded operators from our results. As a consequence, it would be not obvious how to obtain an asymptotic expansion of H' in the norm of bounded operators from the readily available expansion of $\widehat{h}$.

On the other hand the following theorem for H' instead of $\widehat{h}$ would be an obvious consequence of the construction of the previous two sections, while for $\widehat{h}$ a short argument is needed.

Of course, if $\Pi^\varepsilon \widehat{H} \Pi^\varepsilon$ is a bounded operator one can define the effective Hamiltonian through (3.25). This will be done in Chapter 5. ♢

The following theorem is the basis for the adiabatic perturbation theory, as it relates the unitary time-evolution generated by the original Hamiltonian $\widehat{H}$ to the one generated by the effective Hamiltonian $\widehat{h}$.

Theorem 3.20. *Under the assumptions of Theorem 3.12, one has that $h \in S^m_\rho(\varepsilon)$ and $\widehat{h}$ is essentially self-adjoint on $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}})$. Furthermore we have that*

$$[\,\widehat{h},\,\Pi_{\rm r}\,]=0\,, \tag{3.26}$$

$$\mathrm{e}^{-\mathrm{i}\widehat{H}s}-\widehat{u}^{\,*}\,\mathrm{e}^{-\mathrm{i}\widehat{h}s}\,\widehat{u}=\mathcal{O}_0(\varepsilon^\infty|s|) \tag{3.27}$$

and

$$\mathrm{e}^{-\mathrm{i}\widehat{H}s}-U^{\varepsilon\,*}\,\mathrm{e}^{-\mathrm{i}\widehat{h}s}\,U^{\varepsilon}=\mathcal{O}_0(\varepsilon^\infty(1+|s|))\,. \tag{3.28}$$

Remark 3.21. We emphasize that in most applications we will be interested *only* in the effective Hamiltonian restricted to the reference space $\mathcal{K}_{\rm f}$, i.e. in $\Pi_{\rm r}\,\widehat{h}\,\Pi_{\rm r}$. ♢

Proof. Let $\widetilde{h}:=\widehat{u}\,\widehat{H}\,\widehat{u}^*$. Since $\widehat{u}^{\,*}$ is bounded with bounded inverse, one finds, by checking definitions, that $\widetilde{h}$ is self-adjoint on $\widehat{u}^{\,*\,-1}D(\widehat{H})$ and that $\widetilde{h}$ is essentially self-adjoint on $\widehat{u}^{\,*\,-1}\mathcal{S}$. According to Equation (8.10) in [DiSj], which generalizes to $\mathcal{L}(\mathcal{H}_{\rm f})$-valued symbols, $\widehat{u}^{\,*\,-1}\in OPS^0(\varepsilon)$ and thus $\widehat{u}^{\,*\,-1}\mathcal{S}=\mathcal{S}$. Hence $\mathcal{S}(\mathbb{R}^d,\mathcal{H}_{\rm f})$ is a core for $\widetilde{h}$ and, since $\widehat{h}-\widetilde{h}\in\mathcal{L}(\mathcal{H})$, the same conclusions hold true for $\widehat{h}$.

Next observe that, by construction, $[h_j,\pi_{\rm r}]=0$ for all $j\in\mathbb{N}$ and thus $[h_j,\pi_{\rm r}]_\sharp^\sim=0$ because $\pi_{\rm r}$ does not depend on $(q,p)\in\mathbb{R}^{2d}$. Hence $[\widehat{h}_j,\Pi_{\rm r}]=0$ and thus (3.26) follows.

For (3.27) observe that

$$\begin{aligned}&\mathrm{e}^{-\mathrm{i}\widehat{H}s}-\widehat{u}^{\,*}\,\mathrm{e}^{-\mathrm{i}\widehat{h}s}\,\widehat{u}\\&\quad=-\,\mathrm{i}\,\mathrm{e}^{-\mathrm{i}\widehat{H}s}\int_0^s\mathrm{d}s'\,\mathrm{e}^{\mathrm{i}\widehat{H}s'}\left(\widehat{H}\,\widehat{u}^{\,*}-\widehat{u}^{\,*}\widehat{h}\right)\mathrm{e}^{-\mathrm{i}\widehat{h}s'}\,\widehat{u}=\mathcal{O}_0(\varepsilon^\infty|s|)\,,\end{aligned}$$

since, by construction, $(\widehat{H}\,\widehat{u}^{\,*}-\widehat{u}^{\,*}\widehat{h})=\mathcal{O}_0(\varepsilon^\infty)$. Finally (3.28) follows from (3.27) using $U^\varepsilon-\widehat{u}=\mathcal{O}_0(\varepsilon^\infty)$. □

In the remainder of this section we will study the finite order asymptotic approximations

$$\widehat{h}^{(n)}:=\sum_{j=0}^n\varepsilon^j\,\widehat{h}_j$$

to the effective Hamiltonian $\widehat{h}$. By virtue of (3.26), we can, whenever appropriate, restrict our attention to the reduced Hilbert space $\mathcal{K}=\Pi_{\rm r}\mathcal{H}$. Furthermore we define $\widehat{u}^{(n)}=\sum_{j=0}^n\varepsilon^j\,\widehat{u}_j$ and obtain a finite order expansion of the unitary U^ε as $\|\,U^\varepsilon-\widehat{u}^{(n)}\,\|_{\mathcal{L}(\mathcal{H})}=\mathcal{O}(\varepsilon^{n+1})$.

Our main interest are approximations to the solution of the time-dependent Schrödinger equation

$$\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}s}\,\psi(s)=\widehat{H}\,\psi(s) \tag{3.29}$$

over times of order $\varepsilon^{-k}\tau$, where τ does not depend on ε and $k\in\mathbb{N}$ is arbitrary. Expansion of (3.27) on the almost invariant subspace yields the central perturbative result.

Corollary 3.22. *Let $\rho(n+k+1) \geq m$, then for $|s| \leq \varepsilon^{-k}\tau$*

$$\mathrm{e}^{-\mathrm{i}\widehat{H}s}\Pi^\varepsilon = \widehat{u}^{(n)*}\,\mathrm{e}^{-\mathrm{i}\widehat{h}^{(n+k)}s}\,\Pi_{\mathrm{r}}\,\widehat{u}^{(n)} + (1+|\tau|)\mathcal{O}_0(\varepsilon^{n+1})\,. \tag{3.30}$$

Here $\rho(n+k+1) \geq m$ is assumed in order to have $\widehat{h} - \widehat{h}^{(n+k)} \in \mathcal{L}(\mathcal{H})$. Hence, given the level of precision ε^n and the time scale ε^{-k}, the expansion of $\widehat{h}$ must be computed up to order $\widehat{h}_{n+k}$ and the expansion of U^ε up to order $\widehat{u}_n$. Put differently, in order to improve the error, a better approximation to the unitary transformation is necessary. On the other hand, in order to enlarge the time-scale of validity for the space-adiabatic approximation, only the effective Hamiltonian $\widehat{h}$ must be computed to higher orders.

Specializing (3.30) to $n = 0$ and $k = 1$, one obtains the leading order solution of the Schrödinger equation as

$$\mathrm{e}^{-\mathrm{i}\widehat{H}s}\Pi^\varepsilon = \widehat{u}_0^*\mathrm{e}^{-\mathrm{i}(\widehat{h}_0+\varepsilon\widehat{h}_1)s}\,\Pi_{\mathrm{r}}\,\widehat{u}_0 + (1+|\tau|)\mathcal{O}_0(\varepsilon)\,, \quad |s| \leq \varepsilon^{-1}\tau\,, \tag{3.31}$$

where $m \leq 2\rho$. Here the choice of $k = 1$ corresponds to the macroscopic or semiclassical time-scale t/ε. On this time-scale the effective dynamics $\mathrm{e}^{-\mathrm{i}\widehat{h}t/\varepsilon}\Pi_{\mathrm{r}}$ on the reference subspace is expected to have a nice semiclassical limit, under suitable conditions on $\widehat{h}$.

Note that one can replace in (3.30) and analogously in (3.31) τ by $\varepsilon^{-\delta}\tau$ and obtains

$$\mathrm{e}^{-\mathrm{i}\widehat{H}s}\Pi^\varepsilon = \widehat{u}^{(n)*}\mathrm{e}^{-\mathrm{i}\widehat{h}^{(n+k)}s}\,\Pi_{\mathrm{r}}\,\widehat{u}^{(n)} + (1+|\tau|)\mathcal{O}_0(\varepsilon^{n+1-\delta})\,, \quad |s| \leq \varepsilon^{-(k+\delta)}\tau\,. \tag{3.32}$$

Thus one can enlarge the time-span for which the approximation holds without the need to compute further terms in the expansion. The price to be paid is a larger error, of course.

Remark 3.23. We emphasize that (3.30) and (3.31) are purely space-adiabatic expansions with *no semiclassical approximation* invoked yet. As a consequence one obtains uniform results and a simple bound on the growth of the error with time. Note in particular that the space-adiabatic approximation holds on time-scales far beyond the Ehrenfest time-scale, the maximal time-scale for which semiclassical approximations are expected to hold. For some particular cases semiclassical expansions of the full propagator $\mathrm{e}^{-\mathrm{i}\widehat{H}t/\varepsilon}$ have been derived directly, e.g. in the context of the Dirac equation [Ya, BoKe$_2$]. These expansions hold, in general, only for short times, in the sense that they must be modified each time a caustic in the corresponding classical flow is encountered. More important, the clear separation of the space-adiabatic and the semiclassical expansion is not maintained, which is a severe drawback, since in many physical situations the space-adiabatic approximation is valid to high accuracy, while the semiclassical approximation is not, cf. Section 4.1. On the other hand, a semiclassical expansion of the right hand side of (3.31) is straightforward in many interesting cases, as will be discussed in Section 3.4. ♢

Remark 3.24. In parentheses we remark that the space-adiabatic approximation can be used also in the time-independent setting, i.e. to estimate spectral properties of $\widehat{H}$. If one is able to compute eigenvalues of $\widehat{h}^{(n)}$ up to errors of order $o(\varepsilon^n)$,

$$\widehat{h}^{(n)}\,\psi^{(n)} = E^{(n)}\,\psi^{(n)} \,+\, o(\varepsilon^n)\,,$$

it follows that

$$\widehat{H}\,\widehat{u}^*\,\psi^{(n)} = E^{(n)}\,\widehat{u}^*\,\psi^{(n)} \,+\, o(\varepsilon^n)\,.$$

If in addition one knows from some a priori arguments that $\widehat{H}$ has pure point spectrum near $E^{(n)}$, it follows that $\widehat{H}$ has an eigenvalue $o(\varepsilon^n)$-close to $E^{(n)}$. Otherwise one can at least conclude that there is a "resonance" in the sense of a quasi bound state $o(\varepsilon^n)$-close to $E^{(n)}$. We stress that no explicit knowledge of U^ε is needed as long as the interest is in approximate eigenvalues only. For example, the scheme just described can be applied to the time-independent Born-Oppenheimer theory, where one is interested in the low lying spectrum of a molecule. The standard approaches to the time-independent Born-Oppenheimer approximation [CDS, Ha_2, KMSW] yield in some respects mathematically stronger results, cf. Appendix C. However, our scheme suffices for estimating asymptotic expansions of eigenvalues and is simpler to handle, in general. ♢

3.3.1 Expanding the effective Hamiltonian

We turn to the explicit determination of the leading order terms h_j in the expansion of $\widehat{h}$ using (3.24). Of course, in concrete applications only H and u_0 are given explicitly, while the higher order terms in the expansion of u must be calculated using the construction from Section 3.2. For a general Hamiltonian $\widehat{H}$ such a program is feasible only for the terms h_0, h_1 and possibly h_2, which will be our concern in the following.

The principal symbol of h is given by

$$h_0 = u_0\,H_0\,u_0^*\,.$$

Higher order terms can be obtained using (3.24). The double Moyal product becomes rather awkward to handle, and alternatively we proceed inductively by observing that

$$u\,\sharp\,H - h_0\,\sharp\,u = \varepsilon\,h_1\,\sharp\,u + \mathcal{O}(\varepsilon^2) = \varepsilon\,h_1\,u_0 + \mathcal{O}(\varepsilon^2)\,, \tag{3.33}$$

with the subprincipal symbol on the left hand side being

$$(u\,\sharp\,H - h_0\,\sharp\,u)_1 = u_1H_0 + u_0H_1 - h_0u_1 + (u_0\,\sharp\,H_0)_1 - (h_0\,\sharp\,u_0)_1\,. \tag{3.34}$$

Recall the notation $a\,\sharp\,b = \sum_{j=0}^{\infty}\varepsilon^j\,(a\,\sharp\,b)_j$ for the expansion of the Moyal product. Combining (3.33) and (3.34) one obtains

$$h_1 = \big(u_1 H_0 + u_0 H_1 - h_0 u_1 + (u_0 \sharp H_0)_1 - (h_0 \sharp u_0)_1 \big)\, u_0^* \,. \tag{3.35}$$

The expression (3.35) further simplifies if one specializes to the case where $\sigma_*(q,p) = \{E_*(q,p)\}$ consists of a single eigenvalue of $H_0(q,p)$ and one projects on the relevant subspace,

$$\pi_{\mathrm{r}} h_1 \pi_{\mathrm{r}} = \pi_{\mathrm{r}} \big(u_0\, H_1\, u_0^* + (u_0 \sharp H_0)_1\, u_0^* - (E_* \sharp u_0)_1\, u_0^*\big) \pi_{\mathrm{r}} \,. \tag{3.36}$$

The right hand side has the nice property to be independent of u_1 and thus to depend only on known quantities.

Along the same lines and under the same condition on $\sigma_*(q,p)$, one computes

$$\begin{aligned} \pi_{\mathrm{r}} h_2 \pi_{\mathrm{r}} = \pi_{\mathrm{r}} \Big(& u_0 H_2 + u_1 H_1 - h_1 u_1 \\ & + (u_1 \sharp H_0)_1 + (u_0 \sharp H_1)_1 - (E_* \sharp u_1)_1 - (h_1 \sharp u_0)_1 \\ & + (u_0 \sharp H_0)_2 - (E_* \sharp u_0)_2 \Big) u_0^* \pi_{\mathrm{r}} \,. \end{aligned} \tag{3.37}$$

Again, (3.37) does not depend on u_2 for the special case under consideration, but it does depend on u_1, which must now be computed using the construction from Section 3.2.

Although (3.37) looks still rather innocent, in general, it requires some work to compute it explicitly. This is partly because the second order expansion of the Moyal product in (3.37) tends to become rather tedious to obtain. But, in general, also the determination of u_1 is nontrivial. To convince the reader, we state without details that the construction from Sections 3.1 and 3.2 yields

$$u_1^* = u_0^* \Big(-\frac{\mathrm{i}}{4} \{u_0, u_0^*\} + \big[u_0\, \pi_1^{\mathrm{OD}}\, u_0^*, \pi_{\mathrm{r}}\big] + \frac{\mathrm{i}}{4} \big[\big(\{u_0, \pi_0\} u_0^* + u_0 \{\pi_0, u_0^*\} \big), \pi_{\mathrm{r}} \big] \Big) \,, \tag{3.38}$$

with

$$\pi_1^{\mathrm{OD}} = \pi_0 \pi_1 (1 - \pi_0) + (1 - \pi_0) \pi_1 \pi_0 \,,$$

where we used that $(a \sharp b)_1 = -\frac{\mathrm{i}}{2} \{a, b\}$. Recall Definition A.10 of the Poisson bracket $\{\cdot, \cdot\}$.

To compute π_1 from the given quantities one has to use the construction explained in Section 3.1. One finds

$$\begin{aligned} \pi_1^{\mathrm{OD}} = \frac{\mathrm{i}}{2} \big(& R_0(E_*)(1 - \pi_0) \{H_0 + E_*, \pi_0\} \pi_0 \\ & + \pi_0 \{\pi_0, H_0 + E_*\}\, R_0(E_*)\, (1 - \pi_0) \big) \\ & + \pi_0 H_1 R_0(E_*)(1 - \pi_0) + R_0(E_*)(1 - \pi_0) H_1 \pi_0 \,, \end{aligned}$$

where $R_0(E_*)(1 - \pi_0) = (H_0 - E_*)^{-1}(1 - \pi_0)$ is uniformly bounded because of the gap condition. For sake of completeness we mention that

$$\pi_1 = \pi_1^{\mathrm{OD}} - \frac{\mathrm{i}}{2}\left(\pi_0\{\pi_0,\pi_0\}\pi_0 - (1-\pi_0)\{\pi_0,\pi_0\}(1-\pi_0)\right)$$

in this case.

For the higher orders in the expansion of h we only remark that, in general, h_n depends on $u^{(n)}$, $H^{(n)}$ and $h^{(n-1)}$. In the special, but interesting case of an isolated eigenvalue $E_*(q,p)$, h_n depends only on $u^{(n-1)}$, $H^{(n)}$ and $h^{(n-1)}$ and is thus considerably easier to obtain.

Remark 3.25. Note that in the case of $\sigma_*(q,p) = \{E_*(q,p)\}$, the principal symbol $h_0(q,p) = E_*(q,p)\mathbf{1}_{\mathcal{H}_{\mathrm{f}}}$ and the subprincipal symbol $h_1(q,p)$ as given by (3.36) are well defined regardless of the gap condition, provided that the spectral projection $\pi_0(q,p)$ is sufficiently regular. Indeed, we shall find in Chapter 6 that, at least in some special cases, there is still adiabatic decoupling to leading order and an effective dynamics generated by $\widehat{h}_0 + \varepsilon\,\widehat{h}_1$ even without a gap condition . ♢

To get even more explicit formulas for h_1 and h_2, note that in most applications one has no naturally given transformation u_0. Instead one chooses a smooth basis $\{\psi_\alpha(q,p)\}_{\alpha\in I}$ of $\pi_0(q,p)\mathcal{H}_{\mathrm{f}}$ and defines

$$u_0(q,p) = \sum_{\alpha\in I} |\chi_\alpha\rangle\langle\psi_\alpha(q,p)| + r(q,p)$$

where the vectors χ_α form a basis for $\pi_{\mathrm{r}}\mathcal{H}_{\mathrm{f}}$ and $r(q,p)$ is some arbitrary unitary intertwining $\pi_0(q,p)^\perp\mathcal{H}_{\mathrm{f}}$ and $\pi_{\mathrm{r}}^\perp\mathcal{H}_{\mathrm{f}}$. $\pi_{\mathrm{r}}\, h_j(q,p)\,\pi_{\mathrm{r}}$ is independent of the choice of the unitary $r(q,p)$ for all $j \in \mathbb{N}$.

We recall that such a basis $\{\psi_\alpha(q,p)\}_{\alpha\in I}$ of global smooth sections of the bundle over $\mathbb{R}^{2d}$ defined by $\pi_0(q,p)$ always exists, since $\mathbb{R}^{2d}$ is contractible, see Remark 3.17. However, we are not aware of a proof which insures $u_0 \in S^0_\rho$. The situation changes completely, once one considers local domains in the base space which are not contractible. Then it might become necessary to chose as reference space the space of sections of a globally nontrivial bundle.

Assuming that $\sigma_*(q,p) = \{E_*(q,p)\}$ consists of a single eigenvalue of $H_0(q,p)$ of multiplicity ℓ (including $\ell = \infty$), we obtain the $\ell\times\ell$-matrix $\pi_{\mathrm{r}}\, h^{(1)}(q,p)\,\pi_{\mathrm{r}}$ as

$$h^{(1)}_{\alpha\beta} = \langle\chi_\alpha, h^{(1)}\chi_\beta\rangle = E_*\,\delta_{\alpha\beta} + \varepsilon\, h_{1\,\alpha\beta}\,, \tag{3.39}$$

with

$$\begin{aligned} h_{1\,\alpha\beta} &= \langle\chi_\alpha, h_1\chi_\beta\rangle = \langle\psi_\alpha, H_1\psi_\beta\rangle - \tfrac{\mathrm{i}}{2}\,\langle\psi_\alpha, \{(H_0+E_*),\psi_\beta\}\rangle \\ &= \langle\psi_\alpha, H_1\psi_\beta\rangle - \mathrm{i}\langle\psi_\alpha,\, \{E_*,\psi_\beta\}\rangle - \tfrac{\mathrm{i}}{2}\,\langle\psi_\alpha, \{(H_0-E_*),\psi_\beta\}\rangle\,. \end{aligned} \tag{3.40}$$

The indices α and β are matrix-indices, both running from 1 to ℓ. Equations (3.39) and (3.40) are one of our central results. They are still of a simple form and mostly suffice to compute the basic physics. The first term in (3.39) is

referred to as Peierls substitution and the first order correction carries information on the intraband spinor evolution. E.g., as will be discussed in Section 4.1, for the Dirac equation h_1 governs the spin precession. The reason for the particular splitting of the terms in (3.40) will be discussed in Section 3.4.2. Here we only remark that the second term in (3.40) is related to a "generalized" Berry connection. We omit the analogous formula for $h_{2\,\alpha\beta}$, since it is too complicated to be helpful in general.

3.4 Semiclassical limit for effective Hamiltonians

The results of the previous sections are genuine quantum mechanical: semiclassical symbols have been used *only as a tool* in order to construct (and, eventually, to approximate) Π^ε and U^ε. But no attempt was made to approximate the solutions of Schrödinger's equation based on some underlying classical Hamiltonian system, i.e. no semiclassical limit has been performed.

However, under the assumption that $\sigma_{\rm r}(q,p) = \{E_{\rm r}(q,p)\}$ consists of a single eigenvalue of $H_0(q,p)$ of necessarily constant multiplicity ℓ, the principal symbol of $\widehat{h}$ is a scalar multiple of the identity, i.e. $h_0(q,p)\pi_{\rm r} = E_{\rm r}(q,p)\mathbf{1}_{\mathcal{K}_{\rm f}}$, and a semiclassical analysis of $\widehat{h}$ can be done in a standard way using e.g. matrix-valued Wigner transforms or the WKB ansatz. We shall focus on the dynamics of quantum observables, which can be approximated by quantities constructed using only the classical flow Φ^t generated by the (classical, scalar) Hamiltonian $E_{\rm r}(q,p)$. This result is a standard Egorov theorem for matrix-valued observables, see Theorem 3.26. We emphasize that for more general energy bands $\sigma_{\rm r}(q,p)$ one cannot expect a simple semiclassical limit, at least not in the usual sense. Crossings of eigenvalue bands are the most prominent example for such a situation, as mentioned in the "left out topics" section of the introduction and in Section 4.5.

In Section 3.4.2 we shortly comment on the role of the Berry connection for the semiclassical limit of the effective Hamiltonian.

The results of Section 3.4.1 for the semiclassical limit of the effective Hamiltonian in the reference representation are just a straightforward application of standard techniques. However, in our context the solution of Schrödingers equation respectively the observables in the original representation are of physical interest. Hence one needs to translate the results of the semiclassical analysis in the reference representation back to the physical one. This is easy at leading order and discussed in Section 3.4.3. If higher order corrections to the classical flow are taken into account, this change of representation is much less trivial. As a consequence we discuss this point only in the context of concrete applications. In particular we derive the first order corrections to the classical dynamics of physical observables for Dirac particles in Section 4.1.3, and for the Bloch electron in Section 5.3.

3.4.1 Semiclassical analysis for matrix-valued symbols

There are many different approaches to the semiclassical limit in quantum mechanics. We shortly sketch how some of them naturally generalize to matrix-valued Hamiltonians, which appear as effective Hamiltonians in adiabatic perturbation theory.

Egorov's Theorem. Roughly speaking Egorov's theorem states that the quantum mechanical time-evolution of a semiclassical observable is given in good approximation by transporting the symbol of the observable along the classical flow generated by the principal symbol of the Hamiltonian. In the scalar case this follows, as we shall see, directly from the fact (A.11) that the symbol of the commutator of two operators is given, at leading order, through the Poisson bracket of the symbols, i.e.

$$\big[\, a_\varepsilon,\, b_\varepsilon \,\big]_{\widetilde{\sharp}} \asymp -\mathrm{i}\,\varepsilon\,\{\, a_\varepsilon,\, b_\varepsilon \,\} + \mathcal{O}(\varepsilon^3)\,.$$

In the following we will describe how the matrix-character of the symbols changes the picture.

For the moment, we identify $\mathcal{K}_\mathrm{f}$ with $\mathbb{C}^\ell$ and h with $\pi_\mathrm{r}\, h\, \pi_\mathrm{r}$, an $\ell \times \ell$-matrix-valued formal symbol. At least formally, Egorov's theorem is obtained through an expansion of Heisenberg's equations of motion for semiclassical observables: Let $a(q,p,\varepsilon) \in S^0_1(\varepsilon, \mathcal{L}(\mathbb{C}^\ell))$, then the quantum mechanical time evolution of $\widehat{a}$ is given by

$$\widehat{a}(t) = \mathrm{e}^{\mathrm{i}\widehat{h}t/\varepsilon}\,\widehat{a}\,\mathrm{e}^{-\mathrm{i}\widehat{h}t/\varepsilon}$$

and satisfies

$$\frac{\mathrm{d}\,\widehat{a}(t)}{\mathrm{d}t} = \frac{\mathrm{i}}{\varepsilon}\big[\widehat{h},\, \widehat{a}(t)\big]\,. \tag{3.41}$$

Expanding both sides of (3.41) on the level of symbols and using $[E_\mathrm{r}\mathbf{1}, a_n(t)] \equiv 0$, $\mathbf{1} = \mathbf{1}_{\mathbb{C}^\ell}$, one obtains the following hierarchy of equations:

$$\frac{\mathrm{d}\,a_0(t)}{\mathrm{d}t} = \{E_\mathrm{r}\mathbf{1}, a_0(t)\} + \mathrm{i}\,[h_1, a_0(t)] \tag{3.42}$$

$$\frac{\mathrm{d}\,a_1(t)}{\mathrm{d}t} = \{E_\mathrm{r}\mathbf{1}, a_1(t)\} + \mathrm{i}\,[h_1, a_1(t)] + \frac{1}{2}\big(\{h_1, a_0(t)\} - \{a_0(t), h_1\}\big) + \mathrm{i}[h_2, a_0(t)] \tag{3.43}$$

$$\frac{\mathrm{d}\,a_2(t)}{\mathrm{d}t} = \{E_\mathrm{r}\mathbf{1}, a_2(t)\} + \mathrm{i}\,[h_1, a_2(t)] + \dots\,. \tag{3.44}$$

Since $\mathrm{d}a_n(t)/\mathrm{d}t$ does not depend on higher orders, the equations can be solved iteratively. The solution of (3.42) with initial condition $a_0(q,p,0) = a_0(q,p)$ is given through

$$a_0(q,p,t) = D^*(q,p,t)\, a_0(\Phi^t(q,p))\, D(q,p,t)\,, \tag{3.45}$$

where $\Phi^t : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is the solution flow corresponding to the scalar Hamiltonian $E_{\mathrm{r}}(q,p)$. More precisely, $\Phi^t(q_0,p_0) = (q(t),p(t))$, where $(q(t),p(t))$ is the solution of the classical equations of motion

$$\dot{q} = \nabla_p E_{\mathrm{r}}\,, \qquad \dot{p} = -\nabla_q E_{\mathrm{r}}$$

with initial condition (q_0,p_0). $D(q,p,t)$ is the solution of

$$\frac{\partial}{\partial t}\, D(q,p,t) = -\,\mathrm{i}\, h_1(\Phi^t(q,p))\, D(q,p,t)\,. \tag{3.46}$$

with initial condition $D(q,p,0) = \mathbf{1}$. One can think of (3.46) for fixed $(q,p) \in \mathbb{R}^{2d}$ as an equation for the Schrödinger-like unitary evolution induced by the time-dependent Hamiltonian $h_1(\Phi^t(q,p))$ on the Hilbert space $\mathbb{C}^\ell$. Since $h_1(q,p)$ is self-adjoint for all $(q,p) \in \mathbb{R}^{2d}$, the solution $D(q,p,t)$ of (3.46) is unitary for all $(q,p,t) \in \mathbb{R}^{2d} \times \mathbb{R}$.

To see that (3.45) is indeed the solution of (3.42), note that the mappings

$$\mathcal{U}(t) : C_{\mathrm{b}}(\mathbb{R}^{2d}, \mathcal{L}(\mathbb{C}^\ell)) \to C_{\mathrm{b}}(\mathbb{R}^{2d}, \mathcal{L}(\mathbb{C}^\ell))$$

defined through (3.45) for $t \in \mathbb{R}$, i.e.

$$\big(\mathcal{U}(t)\, a_0\big)(q,p) = D^*(q,p,t)\, a_0(\Phi^t(q,p))\, D(q,p,t)\,, \tag{3.47}$$

form a one-parameter group of linear automorphisms on the Banach space $C_{\mathrm{b}}(\mathbb{R}^{2d}, \mathcal{L}(\mathbb{C}^\ell))$, since

$$\begin{aligned}
&\big(\mathcal{U}(t')\,\mathcal{U}(t)\, a_0\big)(q,p) = \\
&\quad = D^*(q,p,t')\, D^*(\Phi^{t'}(q,p),t)\, a_0(\Phi^{t'} \circ \Phi^t(q,p))\, D(\Phi^{t'}(q,p),t)\, D(q,p,t') \\
&\quad = D^*(q,p,t+t')\, a_0(\Phi^{t+t'}(q,p))\, D(q,p,t+t') \\
&\quad = \big(\mathcal{U}(t+t')a_0\big)(q,p)\,.
\end{aligned}$$

Here the group structures of Φ^t and of the solutions of (3.46) are used. Hence $\mathcal{U}(t)$ is a group and it suffices to check that (3.45) solves (3.42) at time $t = 0$, which is easy to see.

Turning to the higher order corrections (3.43), (3.44) etc., they are of the form

$$\frac{\mathrm{d}\, a_n(t)}{\mathrm{d}t} = \{E_{\mathrm{r}}\mathbf{1}, a_n(t)\} + \mathrm{i}[h_1, a_n(t)] + I_n(a_0(t), \ldots, a_{n-1}(t))$$

with an inhomogeneity $I_n(t)$ depending only on the known functions $a_0(t), \ldots, a_{n-1}(t)$. Thus, assuming $a_n(0) = 0$, one finds

$$a_n(t) = \int_0^t \mathrm{d}t'\, \mathcal{U}(t-t')\, I_n(t')\,. \tag{3.48}$$

In order to solve Equation (3.43) for the subprincipal symbol one needs to know h_2. However, if one is interested in semiclassical observables with a

principal symbol which is a scalar multiple of the identity, e.g. in the position $a_0(0) = q\,\mathbf{1}$, the last term in (3.43) vanishes at all times, since, according to (3.45), $a_0(t)$ is a scalar multiple of the identity for all times. In Section 4.1.3 the back reaction of the spin of an electron on its translational motion will be discussed on the basis of (3.43).

We summarize the preceding discussion and state a simple first-order version of Egorov's theorem.

Theorem 3.26. *Let H satisfy either* $\mathbf{(IG)}_m$ *for $m \leq 1$ and $\rho = 1$ or* **(CG)** *with $\rho = 0$. Let $\sigma_{\mathrm{r}}(q,p) = \{E_{\mathrm{r}}(q,p)\}$ be an eigenvalue of $H_0(q,p)$ of finite multiplicity ℓ.*

Then the classical flow Φ^t generated by $E_{\mathrm{r}}(q,p)$ and the solution of (3.46) with initial condition $D(q,p,0) = \mathbf{1}$ exist globally in time. For $a_0 \in S^0_\rho(\mathcal{L}(\mathbb{C}^\ell))$, $a_0(t)$ given by (3.45) is a solution of (3.42) and $a_0(t) \in S^0_\rho(\mathcal{L}(\mathbb{C}^\ell))$ for all $t \in \mathbb{R}$.

For each $T < \infty$ there is a constant $C_T < \infty$ such that for all $t \in [-T,T]$

$$\left\| \mathrm{e}^{\mathrm{i}\widehat{h}t/\varepsilon}\, \widehat{a}_0\, \mathrm{e}^{-\mathrm{i}\widehat{h}t/\varepsilon} \;-\; \widehat{a_0(t)} \right\| \;\leq\; \varepsilon\, C_T\,. \tag{3.49}$$

Proof. Up to the modifications discussed before, the proof follows easily along the lines of Egorov's theorem for scalar valued observables (cf. [Ro, BoRo]): To make the expansion of the Heisenberg equation (3.41) rigorous, note that $E_{\mathrm{r}} = \pi_{\mathrm{r}} h_0 \pi_{\mathrm{r}} \in S^m_\rho(\mathbb{R})$ with $m \leq 1$ and thus the corresponding Hamiltonian vector field is smooth and bounded. It follows by standard ODE techniques [Ro] that $\partial_t a_0(\Phi^t) \in S^0_1$ and hence also $\partial_t a_0(t) \in S^0_1$, where $a_0(t)$ is given by (3.45). Thus one can interchange quantization and differentiation with respect to time and obtains

$$\begin{aligned} a(t) - \widehat{a_0(t)} &= \int_0^t \mathrm{d}t'\, \frac{\mathrm{d}}{\mathrm{d}t'} \left(\mathrm{e}^{\mathrm{i}\widehat{h}t'/\varepsilon}\, \mathcal{W}_\varepsilon(a_0(t-t'))\, \mathrm{e}^{-\mathrm{i}\widehat{h}t'/\varepsilon} \right) \\ &= \int_0^t \mathrm{d}t'\, \mathrm{e}^{\mathrm{i}\widehat{h}t'/\varepsilon} \left(\frac{\mathrm{i}}{\varepsilon} \left[\widehat{h}, \mathcal{W}_\varepsilon(a_0(t-t')) \right] - \mathcal{W}_\varepsilon \left(\frac{\mathrm{d}a_0}{\mathrm{d}t}(t-t') \right) \right) \mathrm{e}^{-\mathrm{i}\widehat{h}t'/\varepsilon}\,. \end{aligned}$$

Now, by construction, $\frac{\mathrm{i}}{\varepsilon} \left[\widehat{h}, \widehat{a_0(t-t')} \right] - \mathcal{W}_\varepsilon \left(\frac{\mathrm{d}a_0}{\mathrm{d}t}(t-t') \right)$ is a semiclassical operator in $\mathrm{OP}S^1_1(\varepsilon)$ with vanishing principal symbol. Hence the integrand is really $\mathcal{O}(\varepsilon)$ as a bounded operator and (3.49) follows. □

There are several results for the scalar case, which hold for more general Hamiltonians, in particular for the usual Schrödinger Hamiltonian, and which contain higher orders, cf. [Ro, BoRo]. Also the matrix-valued version of Egorov's theorem has been discussed several times in the literature [Iv, BrNo, BoGl].

Remark 3.27. Dealing with matrix-valued classical symbols was very natural from the conceptual viewpoint. However, the physical interpretation would

become simpler when one could translate the semiclassical time-evolution of matrix-valued observables given through (3.47) to a (semi)classical time-evolution for states in some appropriate phase space.

An elegant solution to this problem is given by Várilly and Gracia-Bondía [GrVa, VaGr] based on a ideas of Stratonovich [St], who developed a semiclassical calculus for particles with spin. We shortly sketch the construction for later use in the context of the semiclassical limit of the Dirac equation in Section 4.1.3 and refer to Bolte and Glaser [BoGl] for a related application in the context of quantum ergodicity for spinning particles.

Assume that the unitary matrices $D(q,p,t)$ are given via the $(2\ell+1)$-dimensional unitary irreducible representation π_ℓ of $SU(2)$ as $D(q,p,t) = \pi_\ell(d(q,p,t))$ for $d(q,p,t) \in SU(2)$. This is naturally the case if the degeneracy ℓ is related to spin or angular momentum and, as a consequence, $h_1(q,p)$ takes values in the corresponding Lie algebra $\pi_\ell(su(2))$. Then, independently of ℓ, a convenient choice for the classical phase space is $\mathbb{R}^{2d} \times S^2$, since $g \in SU(2)$ acts canonically on S^2 through its projection $\pi(g)$ onto $SO(3)$, i.e. $\pi : SU(2) \to SO(3)$ denotes the covering map. To a matrix valued symbol $A : \mathbb{R}^{2d} \to \mathcal{L}(\mathbb{C}^\ell)$ one associates a scalar symbol on the larger phase space $\mathbb{R}^{2d} \times S^2$ according to

$$a(q,p,n) = \mathrm{Tr}\big(A(q,p)\,\Delta_\ell(n)\big)$$

with a suitable $\Delta_\ell : S^2 \to \mathcal{L}_{\mathrm{sa}}(\mathbb{C}^\ell)$ such that

$$A(q,p) = (2\ell+1)\int_{S^2} \mathrm{d}\lambda(n)\, a(q,p,n)\,\Delta_\ell(n)\,.$$

Here λ denotes normalized Lebesgue measure on S^2. Then the Weyl quantization of a given through

$$(\widehat{a}\varphi)(x) = \frac{2\ell+1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^{2d}}\int_{S^2} \mathrm{d}\xi\,\mathrm{d}y\,\mathrm{d}\lambda(n)\, a\big(\tfrac{1}{2}(x+y),\xi,n\big)\,\mathrm{e}^{\mathrm{i}\xi\cdot(x-y)/\varepsilon}\,\Delta_\ell(n)\,\varphi(y)\,, \tag{3.50}$$

agrees with the one of A, i.e. $\widehat{a} = \widehat{A}$. Most important, one can choose Δ_ℓ such that for $g \in SU(2)$ one has

$$\pi_\ell(g)\,\Delta_\ell(n)\,\pi_\ell(g)^* = \Delta_\ell(\pi(g)\,n)\,.$$

This covariance condition guarantees that (3.47) translates into a flow on phase space $\mathbb{R}^{2d} \times S^2$ as

$$\begin{aligned} a(q,p,n,t) &= \mathrm{Tr}\big(A(q,p,t)\,\Delta_\ell(n)\big) \\ &= \mathrm{Tr}\big(A(\Phi^t(q,p))\,D(q,p,t)\,\Delta_\ell(n)\,D^*(q,p,t)\big) \\ &= \mathrm{Tr}\big(A(\Phi^t(q,p))\,\Delta_\ell(\pi(d(q,p,t))\,n)\big) \\ &= a\big(q(t),p(t),n(t)\big) =: \big(a\circ\Phi_\ell^t\big)(q,p,n)\,. \end{aligned}$$

We will show in Section 4.1.3 how this construction leads to a natural semiclassical limit for the Dirac equation including also back-reaction of the spin-dynamics onto the translational dynamics. ♢

We shortly mention two other approaches, which can be applied to a semiclassical analysis of matrix-valued symbols.

Wigner function. The previous results on the time-evolution of semiclassical observables translate, by the duality expressed through

$$\langle \psi, \, \widehat{a}_0 \, \psi \rangle = \int_{\mathbb{R}^{2d}} \mathrm{d}q \, \mathrm{d}p \, \mathrm{Tr}_{\mathbb{C}^\ell} \left(a_0(q,p) W^\psi(q,p) \right) \, ,$$

to the time-evolution of the Wigner transform

$$W^\psi(q,p) := \mathrm{Symb}(P_\psi)(q,p) = (2\pi)^{-d} \int_{\mathbb{R}^d} \mathrm{d}\xi \, \mathrm{e}^{\mathrm{i}\xi\cdot p} \, \psi(q+\varepsilon\xi/2) \otimes \psi^*(q-\varepsilon\xi/2) \tag{3.51}$$

as

$$\begin{aligned} &\int_{\mathbb{R}^{2d}} \mathrm{d}q \, \mathrm{d}p \, \mathrm{Tr}_{\mathbb{C}^\ell} \left(a_0(q,p) \, W^{\psi_t}(q,p) \right) = \qquad (3.52) \\ &= \int_{\mathbb{R}^{2d}} \mathrm{d}q \, \mathrm{d}p \, \mathrm{Tr}_{\mathbb{C}^\ell} \left(a_0(q,p) \, D^*(q,p,-t) \, W^{\psi_0}(\Phi^{-t}(q,p)) \, D(q,p,-t) \right) + \mathcal{O}(\varepsilon) \, . \end{aligned}$$

Often in (3.52) the limit $\varepsilon \to 0$ is taken, cf. Section 2.3.3, because then the Wigner transform defines a probability measure on phase space and the transport equation looks more classical. Note that this step is not necessary, as one can as well transport the Wigner transform itself along the classical flow. Although it is in general not a positive function, it reproduces correctly the quantum mechanical expectation values. The semiclassical analysis based on matrix-valued Wigner functions and measures was pioneered by Gérard, Markowich, Mauser and Poupaud [GMMP]. For more details on the relation between Egorov type theorems and propagation of Wigner functions see [Te_3].

Semiclassical propagator. Often one is not only interested in the semiclassical propagation of observables, but more directly in a semiclassical expansion of the kernel $K(x,y,t)$ of the unitary group

$$\left(\mathrm{e}^{-\mathrm{i}\widehat{h}t/\varepsilon} \psi \right)(x) = \int_{\mathbb{R}^d} \mathrm{d}y \, K^\varepsilon(x,y,t) \, \psi(y) \, . \tag{3.53}$$

As in the case of Egorov's theorem, generalizing the known results for Hamiltonians with scalar symbols to the case of operator-valued symbols is straightforward, whenever the principal symbol h_0 of h is a scalar multiple of the identity. As in the scalar case, see [Ro], one makes an ansatz of the form

$$K^\varepsilon(x,y,t) = \frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^d} \mathrm{d}p\, \mathrm{e}^{\mathrm{i}\left(S(x,p,t)-y\cdot p\right)/\varepsilon}\Big(\sum_{j=0}^{\infty}\varepsilon^j a_j(x,p,t)\Big)\,,$$

where $S(x,p,t)$ is real valued and the a_j's take values in the bounded linear operators on $\mathbb{C}^\ell$. Demanding (3.53) at time $t=0$, i.e. $K^\varepsilon(x,y,0)=\delta(x-y)$, imposes the following initial conditions on S and $\{a_j\}_{j\geq 0}$:

$$S(x,p,0) = x\cdot p\,, \qquad a_0(x,p,0) = \mathbf{1}_{\mathbb{C}^\ell} \quad \text{and} \quad a_j(x,p,0) = 0 \quad \text{for } j\geq 1\,.$$

For later times the coefficients are determined by formally expanding the Schrödinger equation for $K^\varepsilon(x,y,t)$

$$\mathrm{i}\,\varepsilon\frac{\partial}{\partial t}K^\varepsilon(\cdot,y,t) = \widehat{h}\,K^\varepsilon(\cdot,y,t)$$

in orders of ε. At leading order only $\widehat{h}_0 = \widehat{E}_0$ contributes and one obtains as in the scalar case

$$\partial_t\, S(x,p,t) + E_{\mathrm{r}}\big(x,\nabla_x S(x,p,t)\big) = 0\,, \tag{3.54}$$

the Hamilton-Jacobi equation for the symbol h_0. The next to leading order equation is the so called transport equation for a_0:

$$\mathrm{i}\partial_t a_0(x,p,t) = \mathcal{L}(x,p,t)\,a_0(x,p,t) \,+ h_1\big(x,\nabla_x S(x,p,t)\big)\,a_0(x,p,t)\,. \tag{3.55}$$

The differential operator $\mathcal{L}(x,p,t)$ is the same as in the scalar case, see [Ro] for an explicit formula. Here we just want to point out that the known techniques from the scalar case apply with one modification: as in (3.42), also in (3.55) h_1 contributes as an additional rotation in the transport equation for the leading order term. Since the solution of (3.54) exists only until a caustic is reached, the approximation (3.54), (3.55) to the propagator is a short time result only. The extension to arbitrary times is a complicated task, in general [MaFe].

3.4.2 Geometrical interpretation: the generalized Berry connection

With this preparation we explain the motivation behind the particular splitting of the terms in (3.40). It is of geometrical origin and related to the Berry connection. We will show in Section 4.2 that in the Born-Oppenheimer setting $h_{1\,\alpha\beta}(q,p) = -p\cdot\mathcal{A}_{\alpha\beta}(q)$, a result we obtained already in Chapter 2 for the case of a one-dimensional fibre. Thus $\mathcal{A}_{\alpha\beta}(q)$ acts as a gauge potential of a connection on the trivial bundle $\mathbb{R}^d\times\mathbb{C}^\ell$. Its origin is purely geometrical, since it comes from the connection which the natural connection on the trivial bundle $\mathbb{R}^d\times\mathcal{H}_{\mathrm{f}}\mapsto\mathbb{R}^d$ induces on the subbundle defined by $\pi_0(\cdot)\mathcal{H}_{\mathrm{f}}\mapsto\mathbb{R}^d$. If one assumes that $\pi_0(q)\mathcal{H}_{\mathrm{f}}$ is 1-dimensional, the internal rotations along classical

trajectories are just phase changes, the so called Berry phases, and are due to parallel transport with respect to the Berry connection [Be$_1$, Si, ShWi].

In the general case the second term of $h_{1\,\alpha\beta}(q,p)$ in (3.40), which we denote by

$$h_{\mathrm{Be}\,\alpha\beta}(q,p) = -\mathrm{i}\langle\psi_\alpha(q,p), \{E_\mathrm{r}, \psi_\beta\}(q,p)\rangle,$$

corresponds exactly to this parallel transport along the generalized Berry connection. More precisely, the trivial connection on the trivial bundle $\mathbb{R}^{2d} \times \mathcal{H}_\mathrm{f} \mapsto \mathbb{R}^{2d}$ induces an $U(\ell)$-connection on the subbundle $\pi_0(\cdot,\cdot)\mathcal{H}_\mathrm{f} \mapsto \mathbb{R}^{2d}$. After unitary rotation $u_0(q,p)$ the coefficients of this connection on the bundle $\mathbb{R}^{2d} \times \mathbb{C}^\ell \mapsto \mathbb{R}^{2d}$ are

$$\mathcal{A}_{\alpha\beta}(q,p) = \mathrm{i}\begin{pmatrix} \langle\psi_\alpha(q,p), \nabla_q\psi_\beta(q,p)\rangle \\ \langle\psi_\alpha(q,p), \nabla_p\psi_\beta(q,p)\rangle \end{pmatrix},$$

in the sense that a section $\varphi(q,p)$ is parallel if $(\nabla - \mathrm{i}\mathcal{A})\varphi = 0$. It is parallel along some curve $c(\tau) = \big(q(\tau), p(\tau)\big)$ in $\mathbb{R}^{2d}$ if

$$\Big(\partial_\tau - \dot{c}(\tau)\cdot \mathrm{i}\mathcal{A}\big(q(\tau),p(\tau)\big)\Big)\varphi\big(q(\tau),p(\tau)\big) = 0\,.$$

For classical trajectories, where $\dot{c}(t) = (\nabla_p E_\mathrm{r}, -\nabla_q E_\mathrm{r})^\mathrm{T}$, this condition becomes

$$\Big(\partial_t + \mathrm{i}\,h_\mathrm{Be}\big(q(t),p(t)\big)\Big)\varphi\big(q(t),p(t)\big) = 0\,. \tag{3.56}$$

If $h_1 = h_\mathrm{Be}$, then the spin transport due to h_1, i.e. $\varphi_t\big(q(t),p(t)\big) = D\big(q,p,t\big)\varphi_0$ with D the solution of Equation (3.46), yields solutions of (3.56). Hence, whenever $h_1 = h_\mathrm{Be}$, then the spin dynamics corresponds to parallel transport with respect to the Berry connection along classical trajectories.

Emmrich and Weinstein [EmWe] give a geometric meaning also to the remaining terms in their analog of h_1. While this is a natural venture in the context of geometric WKB approximation, it seems to be less natural in our approach, since we work in a fixed basis in order to obtain simple analytic expressions.

3.4.3 Semiclassical observables and an Egorov theorem

Ultimately the goal is to approximate expectation values of observables in the original Hilbert space $\mathcal{H} = L^2(\mathbb{R}^d, \mathcal{H}_\mathrm{f})$ rather than in $\mathcal{H} = L^2(\mathbb{R}^d, \mathcal{K}_\mathrm{f})$. Before stating a theorem an obvious, but important observation should be made, which seems to have been overlooked, or at least not stressed sufficiently, in related discussions, e.g., [LiFl$_2$, LiWe$_2$, BoKe$_2$, MaSo]: We proved that in the case $\sigma_\mathrm{r}(q,p) = \{E_\mathrm{r}(q,p)\}$ the effective Hamiltonian $\widehat{h}$ projected on the subspace $\mathcal{K} = \Pi_\mathrm{r}\mathcal{H}$ has a semiclassical limit in the sense of a generalized Egorov theorem, in principle, to any order in ε. However, the variables q and p in the rotated representation are *not* the canonical variables of the slow

degrees of freedom in the original problem. More precisely, let $\widehat{q}_{\mathcal{H}} = x \otimes \mathbf{1}_{\mathcal{H}_\mathrm{f}}$ and $\widehat{p}_{\mathcal{H}} = -\mathrm{i}\varepsilon\nabla_x \otimes \mathbf{1}_{\mathcal{H}_\mathrm{f}}$ be the position and momentum operators of the slow degrees of freedom acting on $\mathcal{H}$ and let $\widehat{q}_{\mathcal{K}} = x \otimes \mathbf{1}_{\mathcal{K}_\mathrm{f}}$ and $\widehat{p}_{\mathcal{K}} = -\mathrm{i}\varepsilon\nabla_x \otimes \mathbf{1}_{\mathcal{K}_\mathrm{f}}$ be the same operators acting on $\mathcal{K}$. Then $\widehat{q}_{\mathcal{K}} = U^\varepsilon \, \Pi^\varepsilon \, \widehat{q}_{\mathcal{H}} \, \Pi^\varepsilon \, U^{\varepsilon\,*} + \mathcal{O}(\varepsilon)$ and $\widehat{p}_{\mathcal{K}} = U^\varepsilon \, \Pi^\varepsilon \, \widehat{p}_{\mathcal{H}} \, \Pi^\varepsilon \, U^{\varepsilon\,*} + \mathcal{O}(\varepsilon)$, with a, in general, nonvanishing ε-correction. Indeed the transformation formula (3.40) gives

$$\begin{aligned} \mathrm{Symb}\, U^\varepsilon \, \Pi^\varepsilon \, \widehat{q}_{\mathcal{H}} \, \Pi^\varepsilon \, U^{\varepsilon\,*} &\asymp q + \varepsilon\, \mathrm{i}\langle \psi_\alpha(q,p), \nabla_p \psi_\beta(q,p)\rangle + \mathcal{O}(\varepsilon^2) \\ \mathrm{Symb}\, U^\varepsilon \, \Pi^\varepsilon \, \widehat{p}_{\mathcal{H}} \, \Pi^\varepsilon \, U^{\varepsilon\,*} &\asymp p - \varepsilon\, \mathrm{i}\langle \psi_\alpha(q,p), \nabla_q \psi_\beta(q,p)\rangle + \mathcal{O}(\varepsilon^2)\,, \end{aligned} \tag{3.57}$$

where one uses that E_* in (3.40) was actually h_0. Physically this means that the quantities which behave like position and momentum in the semiclassical limit are only close to the position and momentum of the slow degrees of freedom, but not equal. This phenomenon is well known in the case of the nonrelativistic limit of the Dirac equation. The Newton-Wigner position operator and not the standard position operator goes over to the position operator in the Pauli equation. The standard position operator has neither a nice nonrelativistic limit nor, as we will see, a nice semiclassical limit, because of the Zitterbewegung. Switching to the Newton-Wigner position operator corresponds to averaging over the Zitterbewegung, or, in our language, to use the position operator $\widehat{q}_{\mathcal{K}}$ in the rotated representation. We remark that in the Born-Oppenheimer case, and more generally whenever π_0 depends on q only, one has $\widehat{q}_{\mathcal{K}} = U^\varepsilon \, \Pi^\varepsilon \, \widehat{q}_{\mathcal{H}} \, \Pi^\varepsilon \, U^{\varepsilon\,*} + \mathcal{O}(\varepsilon^2)$.

The following makes precise the connection between observables on the reference space and the original observables at leading order.

Corollary 3.28. *Let $A \in S^0(\mathcal{L}(\mathcal{H}_\mathrm{f}))$, then*

$$U^\varepsilon \, \widehat{A} \, U^{\varepsilon\,*} = \mathcal{W}_\varepsilon(\, u_0 \, A \, u_0^*) + \mathcal{O}_0(\varepsilon)\,.$$

Let $A(q,p) = a(q,p)\,\mathbf{1}_{\mathcal{H}_\mathrm{f}}$ with $a \in S^0(\mathbb{R})$, then

$$U^\varepsilon \, \widehat{A} \, U^{\varepsilon\,*} = \widehat{A} + \mathcal{O}_0(\varepsilon)\,.$$

Proof. Expanding the Moyal products yields

$$\begin{aligned} U^\varepsilon \, \widehat{A} \, U^{\varepsilon\,*} &= \widehat{u} \, \widehat{A} \, \widehat{u}^* + \mathcal{O}_0(\varepsilon^\infty) = \mathcal{W}_\varepsilon(\, u \sharp A \sharp u^*) + \mathcal{O}_0(\varepsilon^\infty) \\ &= \mathcal{W}_\varepsilon(u_0 \, A \, u_0^*) + \mathcal{O}_0(\varepsilon)\,. \end{aligned}$$

For the special case that $A = a\,\mathbf{1}$ we have $\mathcal{W}_\varepsilon(u_0 \, A \, u_0^*) = \mathcal{W}_\varepsilon(A)$. □

Hence, at leading order the Egorov theorem for observables on the reference subspace can be translated back to observables in the original representation.

Corollary 3.29. *Let H satisfy either* $\mathbf{(IG)}_m$ *with $m \leq 1$ and $\rho = 1$ or* **(CG)** *with $\rho = 0$ and let $\sigma_{\mathrm{r}}(q,p) = \{E_{\mathrm{r}}(q,p)\}$ consist of a single eigenvalue of $H_0(q,p)$ of finite multiplicity ℓ. Let $b_0 \in S^0_1(\mathcal{L}(\mathcal{H}_{\mathrm{f}}))$ such that $[b_0, \pi_0] = 0$ and $B(t) := \mathrm{e}^{\mathrm{i}\widehat{H}t/\varepsilon}\,\widehat{b}_0\,\mathrm{e}^{-\mathrm{i}\widehat{H}t/\varepsilon}$. Let $a_0 := \pi_{\mathrm{r}}\,u_0\,b_0\,u_0^*\,\pi_{\mathrm{r}}$ and define $a_0(t)$ is in (3.45). Then for each $T < \infty$ there is a constant $C_T < \infty$ such that for all $t \in [-T,T]$*

$$\big\|\big(B(t) \;-\; \mathcal{W}_\varepsilon(u_0^*\,a_0(t)\,u_0)\big)\Pi^\varepsilon\big\| \;\leq\; \varepsilon\,C_T\,. \tag{3.58}$$

For $b_0 = f\,\mathbf{1}_{\mathcal{H}_{\mathrm{f}}}$, with $f \in S^0_1(\mathbb{R})$, one obtains as a special case of (3.58) that

$$\Big\|\big(B(t) \;-\; \widehat{b_0(\Phi^t)}\big)\Pi^\varepsilon\Big\| \;\leq\; \varepsilon\,C_T\,. \tag{3.59}$$

Corollary 3.29 follows from Theorem 3.26 together with Corollary 3.28.

We conclude this Section with some observations, which are not very deep, but worthwhile to be stated explicitly.

For general observables $B(t) = \mathrm{e}^{\mathrm{i}\widehat{H}t/\varepsilon}\,\widehat{b}_0\,\mathrm{e}^{-\mathrm{i}\widehat{H}t/\varepsilon}$ in the original representation one has semiclassical behavior to any order in the sense of an Egorov theorem if and only if they almost commute with the projection onto the almost invariant subspace, i.e. if

$$\|\,[B(t), \Pi^\varepsilon]\,\| = \|\,[\,\widehat{b}_0\,, \Pi^\varepsilon]\,\| + \mathcal{O}(\varepsilon^\infty) = \mathcal{O}(\varepsilon^\infty)\,. \tag{3.60}$$

However, observables satisfying (3.60) are exactly the pull-backs of semiclassical observables in the reference space, for which, as we argued in Section 3.4.1, an Egorov theorem to arbitrary order can be established. As the bottom line of this remark we thus notice that we obtain all semiclassical observables by restricting our considerations to the reference space.

On the other hand one can take the diagonal part $\Pi^\varepsilon\,B(t)\,\Pi^\varepsilon$ of an arbitrary observable, which then satisfies (3.60) and thus an Egorov theorem to any order. In this way expectation values with respect to initial conditions $\psi_0 \in \Pi^\varepsilon\mathcal{H}$ can be approximated by means of a weak Egorov theorem, since

$$\langle\psi_0,\, B(t)\,\psi_0\rangle = \langle\psi_0,\, \Pi^\varepsilon\,B(t)\,\Pi^\varepsilon\,\psi_0\rangle\,. \tag{3.61}$$

In particular also the original position and momentum operators $\widehat{q}_{\mathcal{H}}$ and $\widehat{p}_{\mathcal{H}}$ satisfy semiclassical equations of motion to arbitrary order if evaluated on states in the range of Π^ε. However, in expectations with respect to general initial conditions the off-diagonal terms will not behave semiclassically and give rise to phenomena like the so called Zitterbewegung of Dirac particles. An important example where we compute higher order corrections to the semiclassical limit of the diagonal parts of $\widehat{q}_{\mathcal{H}}$ and $\widehat{p}_{\mathcal{H}}$ is the semiclassical model of solid states physics presented in Section 5.3.

4 Applications and extensions

Space-adiabatic perturbation theory as developed in Chapter 3 is applicable to many different physical problems. The simplest example which requires the full machinery, i.e. which cannot be solved on the basis of the techniques of Chapter 2, is the Dirac equation with slowly varying external potentials. It is therefore discussed at considerable detail in Section 4.1. However, while the general theory is formally applicable to many interesting physical systems, for rigorous applications extensions are necessary and one must overcome mostly minor technical problems.

It is shown in Section 4.2 how to include Born-Oppenheimer type Hamiltonians, where the growth of the gap as a function of the momentum does not satisfy the conditions of the previous chapter and thus cutoffs for high energies are needed. The generalization to Hamiltonians with symbols in the unbounded operators is left to Chapter 5. However, the basic idea is very simple, as one considers the unbounded operator as a bounded operator from its domain to the full space and applies the symbolic calculus for operators between different Hilbert spaces.

It is also instructive to reconsider the time-adiabatic setting from the point of view of adiabatic perturbation theory, which is done in Section 4.3.

In Section 4.4 we collect several remarks concerning the validity of the adiabatic approximation in concrete applications, where not the asymptotic order of the error but its numerical value are of primary interest. Finally we discuss in Section 4.5 the Born-Oppenheimer approximation near a conical eigenvalue crossing.

4.1 The Dirac equation with slowly varying potentials

In this section we apply adiabatic perturbation theory to the one-particle Dirac equation with slowly varying external potentials. As a result we find that the full Hilbert space $L^2(\mathbb{R}^3, \mathbb{C}^4)$ is the orthogonal sum of two subspaces which are almost invariant under the dynamics. It turns out that the effective Hamiltonians on the two subspaces are associated with electronic respectively positronic dynamics. In Section 4.1.2 we then consider the leading order semiclassical limit of the effective electronic dynamics and deduce, in particular, the T-BMT equation. The latter describes the evolution of a

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spin-vector along the trajectory of a classical relativistic charged point particle subject to external electro-magnetic fields. However, the translational motion itself does not depend on the spin. This example nicely shows that corrections to the effective Hamiltonian beyond leading order carry important physical information.

Finally, we go one step further in Section 4.1.3 and derive higher order corrections to the semiclassical translational motion. The resulting classical equations of motion (4.31) and (4.32) include the relativistic back-reaction of the spin onto the translational dynamics.

4.1.1 Decoupling electrons and positrons

For the convenience of the reader we shortly recall some basic facts about Dirac's equation. We keep track of all physical constants, including $\hbar$, in this section. The Hamiltonian of the one-particle Dirac equation with slowly varying external potentials reads

$$\widetilde{H}_{\mathrm{D}} = c\boldsymbol{\alpha} \cdot \Big(-\mathrm{i}\hbar\nabla_y - \frac{e}{c}A(\varepsilon y)\Big) + \boldsymbol{\beta}mc^2 + e\phi(\varepsilon y)$$

and acts on $L^2(\mathbb{R}^3, \mathbb{C}^4)$. Here $A : \mathbb{R}^3 \to \mathbb{R}^3$ is the vector potential of an external magnetic field $B = \nabla \times A$ and $\phi : \mathbb{R}^3 \to \mathbb{R}$ the potential of an external electric field $E = -\nabla\phi$. For the Dirac matrices $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$ we chose the standard representation

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \qquad \boldsymbol{\beta} = \begin{pmatrix} \mathbf{1}_{\mathbb{C}^2} & 0 \\ 0 & -\mathbf{1}_{\mathbb{C}^2} \end{pmatrix},$$

where $\boldsymbol{\sigma} = (\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3)$ denotes the vector of the Pauli spin matrices defined in (1.48). For better readability we use boldface letters for 2×2 matrices in this section. The small parameter $\varepsilon > 0$ controls the variation of the external potentials.

Remark 4.1. In their famous paper [FoWo] Foldy and Wouthuysen consider the non-relativistic limit $\frac{v}{c} \ll 1$ of the Dirac equation. They show that the electronic and the positronic subspaces decouple at any order in the asymptotic expansion with respect to $\frac{v}{c}$. At leading order they find the Pauli Hamiltonian as the effective Hamiltonian for a non-relativistic electron and at higher orders they obtain the celebrated relativistic corrections. While Foldy and Wouthuysen show that electrons and positrons decouple in the limit of small velocities, our analysis will show that electrons and positrons decouple in the limit of weak fields. In this sense our resulting effective Hamiltonian (4.9) for an electron can be thought of as a relativistic Pauli Hamiltonian. ♢

In contrast to the discussion in Section 1.2.2 we will work in the position representation and switch to the macroscopic space-scale $x = \varepsilon y$. On this scale the Dirac Hamiltonian becomes

$$\widehat{H}_{\mathrm{D}} = c\boldsymbol{\alpha} \cdot \left(-\mathrm{i}\varepsilon\hbar\nabla_x - \frac{e}{c}A(x)\right) + \boldsymbol{\beta}mc^2 + e\phi(x)\,. \tag{4.1}$$

We are interested in the solution of the time-dependent Dirac equation

$$\mathrm{i}\,\varepsilon\hbar\frac{\partial}{\partial t}\psi(t) = \widehat{H}_{\mathrm{D}}\,\psi(t) \tag{4.2}$$

for $|t| = \mathcal{O}(1)$ or even larger time scales. The solutions of (4.2) for small ε approximately describe the dynamics of electrons, resp. positrons, in weak fields, as in storage rings, accelerators, or cloud chambers, for example.

The Dirac Hamiltonian $\widehat{H}_{\mathrm{D}}$ is the Weyl quantization of the matrix-valued function

$$H_{\mathrm{D}}(q,p) = c\boldsymbol{\alpha} \cdot \left(p - \frac{e}{c}A(q)\right) + \boldsymbol{\beta}mc^2 + e\phi(q)$$

on phase space $\mathbb{R}^6$, where now Weyl quantization is in the sense of $p \mapsto -\mathrm{i}\varepsilon\hbar\nabla_x$, i.e. on the right hand side of (A.4) ε must be replaced by $\varepsilon\hbar$. Planck's constant $\hbar$ appears here for dimensional reasons and is a fixed physical constant. The small parameter of the space-adiabatic expansion is ε, the variation of the external potentials. Notation becomes simpler if we introduce the kinetic momentum

$$k(q,p) := p - \tfrac{e}{c}\,A(q)\,.$$

The symbol-matrix $H_{\mathrm{D}}(q,p)$ has two two-fold degenerate eigenvalues

$$E_{\pm}(q,k) = \pm E_0(k) + e\phi(q)$$

with the corresponding eigenprojections

$$P_{\pm}(k) = \frac{1}{2}\left(1 \pm \frac{c}{E_0(k)}\,(\boldsymbol{\alpha}\cdot k + \boldsymbol{\beta}mc)\right)\,,$$

where $E_0(k) = c\sqrt{m^2c^2 + k^2}$, cf. Figure 1.3. Obviously

$$E_+(q,k(q,p)) - E_-(q,k(q,p)) = 2E_0(p - \tfrac{e}{c}A(q)) \geq C\langle p\rangle > 0\,,$$

whenever A is uniformly bounded. Therefore the corresponding subspaces are adiabatically decoupled and the effective dynamics on each of them can be computed using the general scheme of Chapter 3. Assuming $A \in C^\infty_{\mathrm{b}}(\mathbb{R}^3,\mathbb{R}^3)$ and $\phi \in C^\infty_{\mathrm{b}}(\mathbb{R}^3,\mathbb{R})$, one finds that $H_0 \in S^1_1$ and thus Assumption $(\mathrm{IG})_1$ from Chapter 3 is satisfied. Furthermore, according to Proposition A.8, $\widehat{H}_{\mathrm{D}}$ is essentially self-adjoint on $\mathcal{S}(\mathbb{R}^4,\mathbb{C}^4)$ and $\widehat{E}_{\pm}$ are essentially self-adjoint on $\mathcal{S}(\mathbb{R}^4)$.

To be consistent with the notation of the previous chapter, let $\pi_0(k(q,p))= P_+(k(q,p))$ be the projector on the electron band. The reference subspace for the electrons is $\mathcal{K} = L^2(\mathbb{R}^3,\mathbb{C}^2)$ and it is convenient to define it as the range of

$$\Pi_{\mathrm{r}} := \begin{pmatrix} \mathbf{1}_{\mathbb{C}^2} & 0 \\ 0 & 0 \end{pmatrix}$$

in $L^2(\mathbb{R}^3, \mathbb{C}^4)$.

The only choice left is the one of $u_0(q,p)$ or, equivalently, of a basis $\{\psi_\alpha(q,p)\}_{\alpha=1,2}$ of $\pi_0(k(q,p))\mathbb{C}^4$. Since the degeneracy of $\pi_0(k)\mathbb{C}^4$ is related to the spin of the electron, a natural choice is the $\boldsymbol{\sigma}_z$-representation with respect to the "mean"-spin $\mathbf{S}(k)$ which commutes with $H_{\mathrm{D}}(q,k)$ [FoWo, Th]. The eigenvectors $\psi_\pm(k)$ of the operator $e_3 \cdot \mathbf{S}(k)$ in $\pi_0(k)\mathbb{C}^4$ are

$$\psi_+(k) = \frac{1}{\sqrt{2E_0(k)(E_0(k)+mc^2)}} \begin{pmatrix} E_0(k)+mc^2 \\ 0 \\ ck_3 \\ c(k_1+ik_2) \end{pmatrix} \tag{4.3}$$

$$= \sqrt{\frac{E_0(k)}{2(E_0(k)+mc^2)}} \begin{pmatrix} E_0(k)^{-1}(E_0(k)+mc^2) \\ 0 \\ v_3(k)/c \\ (v_1(k)+iv_2(k))/c \end{pmatrix}$$

and

$$\psi_-(k) = \frac{1}{\sqrt{2E_0(k)(E_0(k)+mc^2)}} \begin{pmatrix} 0 \\ E_0(k)+mc^2 \\ c(k_1-ik_2) \\ -ck_3 \end{pmatrix} \tag{4.4}$$

$$= \sqrt{\frac{E_0(k)}{2(E_0(k)+mc^2)}} \begin{pmatrix} 0 \\ E_0(k)^{-1}(E_0(k)+mc^2) \\ (v_1(k)-iv_2(k))/c \\ -v_3(k)/c \end{pmatrix}.$$

Here we introduced the velocity $v(k) := c^2\, k/E_0(k)$ in order to illustrate that the lower components of $\psi_\pm(k)$ vanish in the non-relativistic limit $v \ll c$. The relevant part of u_0 for the analysis of the electron band is thus given by $u_0^*(k) = \big(\psi_+(k), \psi_-(k), *, *\big)$ with $u_0 \in S_1^0$. Of course the positron part indicated by $*$'s would be given through charge conjugation. In our construction we want to emphasize, however, that no specification is needed in order to determine the expansion of the effective electron Hamiltonian $\widehat{h}_{\mathrm{e}} := \Pi_{\mathrm{r}}\, \widehat{h}\, \Pi_{\mathrm{r}}$ up to arbitrary order.

An alternative way to arrive at the same $u_0(q,p)$ is to note that the Foldy-Wouthuysen transformation $u_{\mathrm{FW}}(p)$, c.f. [FoWo], diagonalizes the free Dirac Hamiltonian $H_0(p)$, i.e. H_{D} with $A, \phi \equiv 0$. Including the fields $u_0(q,p) = u_{\mathrm{FW}}(p - \frac{e}{c}A(q))$ then diagonalizes $H_{\mathrm{D}}(q,p)$.

For the principal symbol of the effective electron Hamiltonian $\widehat{h}_{\mathrm{e}}$ one finds of course

$$h_{\mathrm{e},0}(q,p) = E_+(q, k(q,p))\mathbf{1}_{\mathbb{C}^2}\,.$$

For the subprincipal symbol after a lengthy but straightforward calculation our basic formula (3.40) yields

$$
\begin{aligned}
&h_{\mathrm{e},1}(q,p) = \\
&= -\frac{\hbar ec}{2E_0(k(q,p))}\,\boldsymbol{\sigma}\cdot\left(B(q) - \frac{E_0(k(q,p))}{c\,(E_0(k(q,p))+mc^2)}\,v(k(q,p))\times E(q)\right) \\
&=: -\frac{\hbar}{2}\,\boldsymbol{\sigma}\cdot\Omega(q,k(q,p))\,. \qquad (4.5)
\end{aligned}
$$

Note that the factor $\hbar$ comes from the fact that the n^{th} term in the space-adiabatic expansion carries a prefactor $\hbar^n$. Defining

$$\gamma(k) = 1/\sqrt{1-(v(k)/c)^2} = E_0(k)/(mc^2)$$

one can rewrite

$$\Omega(q,k) = \frac{e}{mc}\left(\frac{1}{\gamma(k)}\,B(q) - \frac{1}{(1+\gamma(k))}\,\frac{v(k)}{c}\times E(q)\right). \qquad (4.6)$$

Remark 4.2. The expression (4.6) for Ω is well known as the frequency appearing in the T-BMT equation, see Section 4.1.2. Here we only note that it yields the Pauli equation in the non-relativistic limit $v \ll c$,

$$\Omega_{\mathrm{Pauli}}(q,k) = \frac{e}{mc}\left(B(q) - \frac{1}{2}\,\frac{v(k)}{c}\times E(q)\right),$$

including the correct spin-orbit coupling as the first relativistic correction. ♢

Remark 4.3. For later use and since the computation leading to (4.5) is not entirely painless, we note that as an important intermediate step one finds for the Berry connection that

$$\mathcal{A}(k)_{\alpha\beta} = \mathrm{i}\hbar\langle\psi_\alpha(k),\nabla_k\psi_\beta(k)\rangle = -\frac{\hbar c^2\,(\boldsymbol{\sigma}\times k)_{\alpha\beta}}{2E_0(k)(E_0(k)+mc^2)} = -\frac{\hbar\,(\boldsymbol{\sigma}\times v(k))_{\alpha\beta}}{2mc^2(1+\gamma(k))}$$

where $\alpha,\beta\in\{+,-\}$. In matrix notation this becomes

$$\boldsymbol{\mathcal{A}}(k) = -\frac{\hbar c^2}{2E_0(k)(E_0(k)+mc^2)}\,\boldsymbol{\sigma}\times k = -\frac{\hbar}{2mc^2(1+\gamma(k))}\,\boldsymbol{\sigma}\times v(k)\,.$$

Hence we can rewrite $h_{\mathrm{e},1}$ in the form

$$h_{\mathrm{e},1}(q,p) = -\mathbf{M}(k)\cdot B(q) - e\,\boldsymbol{\mathcal{A}}(k)\cdot E(q)\,, \qquad (4.7)$$

where

$$\mathbf{M}(k) = \frac{\hbar ec}{2E_0(k)}\,\boldsymbol{\sigma}\,.$$

This expression for h_1 will turn out useful when we determine the corrections to the semiclassical limit of the translational motion in Section 4.1.3. For the analysis of the spin dynamics in Section 4.1.2 the expression (4.5) is more convenient. ♢

We summarize our results on the adiabatic decoupling and the effective dynamics for the Dirac equation in the following

Theorem 4.4. *Let $A \in C_{\mathrm{b}}^{\infty}(\mathbb{R}^3, \mathbb{R}^3)$ and $\phi \in C_{\mathrm{b}}^{\infty}(\mathbb{R}^3, \mathbb{R})$. Then there exist orthogonal projectors $\Pi_{\pm}^{\varepsilon}$ with $\Pi_{+}^{\varepsilon} + \Pi_{-}^{\varepsilon} = \mathbf{1}$ such that $[\widehat{H}_{\mathrm{D}}, \Pi_{\pm}^{\varepsilon}] = \mathcal{O}_0(\varepsilon^{\infty})$, and there exists a unitary U^{ε} and $\widehat{h} \in \mathrm{OP}S_1^1$ with*

$$\widehat{h} = \begin{pmatrix} \widehat{h}_{\mathrm{e}} & 0 \\ 0 & \widehat{h}_{\mathrm{p}} \end{pmatrix},$$

such that

$$\mathrm{e}^{-\mathrm{i}\widehat{H}_{\mathrm{D}} s} - U^{\varepsilon *}\, \mathrm{e}^{-\mathrm{i}\widehat{h} s}\, U^{\varepsilon} = \mathcal{O}_0(\varepsilon^{\infty}(1 + |s|)). \tag{4.8}$$

Here $\widehat{h}_{\mathrm{e}}$ and $\widehat{h}_{\mathrm{p}}$ are semiclassical operators on $L^2(\mathbb{R}^3, \mathbb{C}^2)$ with

$$h_{\mathrm{e}}(q, p, \varepsilon) \asymp E_{+}(q, p)\mathbf{1}_{\mathbb{C}^2} + \sum_{j=1}^{\infty} \varepsilon^j\, h_{\mathrm{e},j}(q, p)$$

and

$$h_{\mathrm{e},j} = \pi_{\mathrm{r}}(u \sharp H_{\mathrm{D}} \sharp u^*)_j \pi_{\mathrm{r}} \in S_1^{1-j}(\mathcal{L}(\mathbb{C}^2))$$

for all $j \geq 0$, where $u \in S_1^0(\varepsilon)$ is constructed as in Section 3.2. In particular, $h_{\mathrm{e},1}(q, p)$ is given by (4.5) and thus the "relativistic Pauli Hamiltonian" is

$$\widehat{h}_{\mathrm{e}} = \Big(c\sqrt{m^2c^2 + (-i\varepsilon\hbar\nabla_x - \frac{e}{c}A(x))^2} + e\phi(x)\Big)\mathbf{1}_{\mathbb{C}^2} \; - \; \varepsilon\,\frac{\hbar}{2}\,\boldsymbol{\sigma}\cdot\Omega(x, -\mathrm{i}\varepsilon\hbar\nabla_x) + \mathcal{O}_0(\varepsilon^2). \tag{4.9}$$

Analogous results hold for h_{p}. The errors in (4.8) and (4.9) are in the norm of bounded operators on $L^2(\mathbb{R}^3, \mathbb{C}^4)$, resp. on $L^2(\mathbb{R}^3, \mathbb{C}^2)$.

According to the effective Hamiltonian (4.9) the g-factor of the electron equals 2. There would be no problem to add to the Dirac Hamiltonian the standard subprincipal symbol [Th], which accounts for the slightly larger g-factor of real electrons. Blount [Bl$_3$] computes the second order effective Hamiltonian $h_{\mathrm{e},2}$, which he finds to be proportional to $\mathbf{1}_{\mathbb{C}^2}$. $h_{\mathrm{e},2}$ is a sum of terms allowed by dimensional reasoning, i.e. proportional to ∇B, ∇E, B^2, E^2, EB. Second order corrections seem to be of interest for the dynamics of electrons in storage rings. Ignoring the contribution [Bl$_3$], non-rigorous expansions were given in [DeKo] and [HeBa]. Finally also Cordes [Cor$_1$, Cor$_2$] constructs a "semiclassical Foldy-Wouthuysen transformation", which matches exactly our transformation u and derives from this an algebra of "predictable observables" for the Dirac equation. The the latter is given through the algebra of those semiclassical observables, which almost commute with $\Pi_{\pm}^{\varepsilon}$.

Remark 4.5. As to be explained in Section 4.3, adiabatic perturbation theory can be extended in order to also allow for time-dependent external potentials in the Dirac equation, cf. Remark 4.16. The only change in the effective Hamiltonian—apart from all potentials being time-dependent—is that the electric field $E(q,t) = -\nabla\phi(q,t)$ in the expression (4.5) for its subprincipal symbol is replaced by $E(q,t) + \dot{A}(q,t)/c$. This follows from inserting (4.3) and (4.4) into Equation (4.44) and a straightforward calculation. ♢

4.1.2 Semiclassical limit for electrons: the T-BMT equation

Equipped with $h_{\mathrm{e},0}$ and $h_{\mathrm{e},1}$ we can apply the general results discussed in Section 3.4 to the semiclassical limit of the Dirac equation. We first consider the translational dynamics, i.e. the dynamics of scalar observables. Let $\Phi_{\pm}^t$ be the Hamiltonian flows generated by the relativistic energy functions

$$E_{\pm}(q,p) = \pm c\sqrt{mc^2 + \big(p - \tfrac{e}{c}A(q)\big)^2}$$

on phase space $\mathbb{R}^6$. Then from Corollary 3.29 we immediately obtain the following result.

Proposition 4.6. *Let $\widehat{B} = \widehat{b}\,\mathbf{1}_{\mathbb{C}^4}$, $b \in S_1^0(\mathbb{R})$, i.e. a semiclassical observable in the original representation which does not test spin. Then for each $T < \infty$ there exists a constant C_T such that for all $t \in [-T,T]$*

$$\Big\| \Big(\mathrm{e}^{\mathrm{i}\widehat{H}_{\mathrm{D}}t/(\varepsilon\hbar)}\, \widehat{B}\, \mathrm{e}^{-\mathrm{i}\widehat{H}_{\mathrm{D}}t/(\varepsilon\hbar)} - \widehat{b\circ\Phi_+^t}\,\mathbf{1}_{\mathbb{C}^4} \Big) \Pi_+^\varepsilon \Big\| \leq \varepsilon\, C_T \tag{4.10}$$

and

$$\Big\| \Big(\mathrm{e}^{\mathrm{i}\widehat{H}_{\mathrm{D}}t/(\varepsilon\hbar)}\, \widehat{B}\, \mathrm{e}^{-\mathrm{i}\widehat{H}_{\mathrm{D}}t/(\varepsilon\hbar)} - \widehat{b\circ\Phi_-^t}\,\mathbf{1}_{\mathbb{C}^4} \Big) \Pi_-^\varepsilon \Big\| \leq \varepsilon\, C_T\,. \tag{4.11}$$

Hence, to leading order, states in the range of Π_+^ε behave like classical relativistic electrons and states in the range of Π_-^ε like classical relativistic positrons. We emphasize that, in general, $\Pi_\pm^\varepsilon$ are not spectral projections of $\widehat{H}_{\mathrm{D}}$, since the variation of ϕ can be larger than the mass gap $2mc^2$. Hence in the limit of slowly varying potentials a natural characterization of "electronic" and "positronic" subspaces is obtained which does *not* come from spectral projections of the free or full Dirac Hamiltonian.

Next we discuss the leading order spin dynamics, which in the first place requires to figure out which operator represents the spin of the electron. There has been a considerable discussion on this point, cf. [Th], with no general consensus reached. We suspect that the problem is void. The wave function is spinor valued and what is observed is the spatial splitting of different spinor components in inhomogeneous magnetic fields. Hence we should pick the "spin observable" Σ such that the splitting can nicely be attributed to it. E.g., in a magnetic field with gradient along the z-direction the eigenvectors of Σ_z should have the property that their spatial support goes either parallel

to $+z$ or to $-z$, but should not split. In view of (4.9) a natural choice is to take as spin operator the vector of Pauli-matrices $\boldsymbol{\sigma}$ in the electronic reference subspace. In the original Hilbert space this amounts to

$$\Sigma = U^{\varepsilon\,*} \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix} U^{\varepsilon} = \frac{2}{\hbar}\,\widehat{S} + \mathcal{O}(\varepsilon)\,,$$

where $S(q,p)$ is the "mean" spin defined before.

The leading order semiclassical approximation for

$$\boldsymbol{\sigma}(t) = \mathrm{e}^{\mathrm{i}\widehat{h}_{\mathrm{e}}t/(\varepsilon\hbar)}\,\boldsymbol{\sigma}\,\mathrm{e}^{-\mathrm{i}\widehat{h}_{\mathrm{e}}t/(\varepsilon\hbar)}$$

follows from Theorem 3.26. For each $T < \infty$ there is a constant $C_T < \infty$ such that for $t \in [-T, T]$

$$\left\| \boldsymbol{\sigma}(t) - \widehat{\boldsymbol{\sigma}_0(t)} \right\| \leq \varepsilon\, C_T\,,$$

where $\boldsymbol{\sigma}_{0k}(q,p,t)$, $k \in \{1,2,3\}$, is obtained as the solution of

$$\frac{\partial\, \boldsymbol{\sigma}_{0k}(q,p,t)}{\partial t} = -\,\frac{\mathrm{i}}{2}\,\Big[\, \boldsymbol{\sigma} \cdot \Omega(\Phi_+^t(q,p)),\, \boldsymbol{\sigma}_{0k}(q,p,t) \,\Big] \tag{4.12}$$

with initial condition $\boldsymbol{\sigma}_{0k}(q,p,0) = \boldsymbol{\sigma}_k$. This follows from the Equations (3.45) and (3.46) by setting $\boldsymbol{\sigma}_{0k}(q,p,t) = D^*(q,p,t)\,\boldsymbol{\sigma}_k\,D(q,p,t)$.

To solve Equation (4.12) one makes an ansatz $\boldsymbol{\sigma}_{0k}(q,p,t) = s_k(q,p,t)\cdot\boldsymbol{\sigma}$ with $s_k(q,p,0) = e_k$. Using $[\boldsymbol{\sigma}_n, \boldsymbol{\sigma}_m] = 2\,\mathrm{i}\,\varepsilon_{nmk}\,\boldsymbol{\sigma}_k$, one finds that the spinor "magnetization"-vector $s_k(q,p,t)$ is given as the solution of

$$\frac{\partial\, s_k(q,p,t)}{\partial t} = -\,s_k(q,p,t)\;\times\;\Omega(\Phi_+^t(q,p))\,. \tag{4.13}$$

Equation (4.13) is the T-BMT equation [Tho, BMT, Ja] on the level of observables. It was derived by Thomas and, in a more general form, by Bargmann, Michel and Telegdi on purely classical grounds as the simplest Lorentz invariant equation for the spin dynamics of a classical relativistic particle. For definiteness we repeat the result as a corollary.

Corollary 4.7. *Let $s_k(q,p,t)$ be the solution of the T-BMT equation (4.13) with initial condition $s_k(q,p,0) \equiv e_k$. Then for each $T < \infty$ there is a $C_T < \infty$ such that for all $t \in [-T,T]$*

$$\left\| \left(\mathrm{e}^{\mathrm{i}\widehat{H}_{\mathrm{D}}t/(\varepsilon\hbar)}\,\widehat{S}_k\,\mathrm{e}^{-\mathrm{i}\widehat{H}_{\mathrm{D}}t/(\varepsilon\hbar)} - \frac{\hbar}{2}\,\widehat{s_k(t)}\cdot\widehat{S} \right) \Pi_+^{\varepsilon} \right\| \leq \varepsilon\, C_T$$

and an analogous result holds for the positronic subspace.

The semiclassical limit of the Dirac equation has been discussed repeatedly and we mention only some recent work. Yajima [Ya] considers time-dependent external fields and proves directly a semiclassical expansion for the

corresponding propagator. As mentioned already at the end of Section 3.4.1, this program is mathematically rather involved, since one faces the problem of caustics in the classical flow, and different expansions have to be glued together in order to obtain results valid for all macroscopic times. Another treatment of the same approach is given by Bolte and Keppeler [BoKe$_2$], who derive a Gutzwiller type trace formula. Since $\widehat{H}_{\mathrm{D}}$ and $U^\varepsilon\,\widehat{H}_{\mathrm{D}}\,U^{\varepsilon\,*}$ are isospectral and since (4.8) holds, a trace formula for the eigenvalue statistics of $\widehat{H}_{\mathrm{D}}$ could as well be derived from the semiclassical propagator of $\widehat{h} = \widehat{h}_{\mathrm{e}} \otimes \mathbf{1} + \mathbf{1} \otimes \widehat{h}_{\mathrm{p}}$. As argued in Section 3.4, the latter is somewhat easier to obtain. In [GMMP, Sp$_1$] the semiclassical limit of the Dirac equation is discussed using matrix-valued Wigner functions.

While Proposition 4.6 and Corollary 4.7 are completely satisfactory formulations of the leading order semiclassical limit for Dirac electrons, we now discuss an alternative formulation based on the scheme introduced in Remark 3.27. At leading order this formulation will not give much new insight, however, it allows us to better incorporate higher order corrections into the classical flow. In the next section we shall see that, in particular, the back-reaction of the spin onto the translational dynamics becomes visible at subleading order, hence our interest.

In the case of the Dirac electron an alternative natural framework for the formulation of the semiclassical limit in the electronic reference representation is that of the classical flow Φ_ℓ^t on phase space $\mathbb{R}^{2d} \times S^2$ described in Remark 3.27. In the present case we have $\ell = \frac{1}{2}$ and

$$\Delta_{\frac{1}{2}}(n) = \frac{1}{2}\mathbf{1}_{\mathbb{C}^2} + \sqrt{\frac{3}{4}}\, n \cdot \boldsymbol{\sigma}$$

satisfies all the conditions of Remark 3.27, cf. [BGK]. Recall that in this setting one associates with a matrix-valued symbol $A(q,p) \in \mathcal{L}(\mathbb{C}^2)$ a scalar symbol $a(q,p,n)$ through

$$a(q,p,n) = \operatorname{Tr} A(q,p)\, \Delta_{\frac{1}{2}}(n)$$

and conversely

$$A(q,p) = 2 \int_{S^2} \mathrm{d}\lambda(n)\, a(q,p,n)\, \Delta_{\frac{1}{2}}(n)\,,$$

where λ denotes the normalized Lebesgue measure on S^2. One finds that the symbol of $\boldsymbol{\sigma}$ is $\sqrt{3}n$.

Now one can define the classical flow $\Phi_0^t : \mathbb{R}^6 \times S^2 \to \mathbb{R}^6 \times S^2$ on the extended phase space as the flow of the vector field

$$\dot{q} = \nabla_p E_+(q,p)\,, \quad \dot{p} = -\nabla_q E_+(q,p)\,, \quad \dot{n} = n \times \Omega(q,p)\,. \tag{4.14}$$

The flow Φ_0^t has the special structure that $q(t)$ and $p(t)$ are independent of n, hence the spin degree of freedom does not influence the translational degrees

of freedom and $\Phi_0^t(q(t),p(t),n(t)) = \big(\Phi_+^t(q,p),n(t)\big)$, where $n(t)$ solves the T-BMT equation

$$\dot{n} = n \times \Omega(\Phi_+^t(q,p)) \tag{4.15}$$

along the prescribed trajectories $\Phi_+^t(q,p)$. More technically speaking, Φ_0^t is a skew-product flow, cf. [BGK]. According to Remark 3.27 we have the following Egorov theorem for observables in the reference space.

Corollary 4.8. *Let $a \in C^\infty(\mathbb{R}^6 \times S^2)$ such that $a(\cdot,\cdot,n) \in S_1^0(\mathbb{R})$ for all $n \in S^2$. Then for all $T < \infty$ there is a constant $C_T < \infty$ such that for all $t \in [-T,T]$*

$$\| \mathrm{e}^{\mathrm{i}\widehat{h}_{\mathrm{e}}t/(\varepsilon\hbar)}\, \widehat{a}\, \mathrm{e}^{-\mathrm{i}\widehat{h}_{\mathrm{e}}t/(\varepsilon\hbar)} - \widehat{a \circ \Phi_0^t} \| \leq \varepsilon\, C_T\,. \tag{4.16}$$

Proof. This is a direct consequence of Theorem 3.26 and Remark 3.27. □

The analogous skew-product Egorov theorem for Pauli Hamiltonians is proved in [BGK] and in a more general setting in [BoGl].

As long as we are interested in the leading order behavior, it is again straightforward to translate the result to the original representation. Let

$$\Delta_{\frac{1}{2}}^\varepsilon(q,p,n) = u^* \sharp \Delta_{\frac{1}{2}}(n) \sharp u\,,$$

where u is the symbol of the unitary U^ε, then for $A \in S_1^0(\mathbb{C}^2)$ we have that

$$\begin{aligned}
\mathrm{Symb}\, U^{\varepsilon\,*}\, \widehat{A}\, U^\varepsilon &= u^* \sharp A \sharp u \\
&= 2 \int_{S^2} \mathrm{d}\lambda(n)\, u^* \sharp a(n)\, \Delta_{\frac{1}{2}}(n) \sharp u \\
&= 2 \int_{S^2} \mathrm{d}\lambda(n)\, u^* \sharp a(n) \sharp u \sharp \Delta_{\frac{1}{2}}^\varepsilon(n) \\
&= 2 \int_{S^2} \mathrm{d}\lambda(n)\, a(q,p,n)\, \Delta_{\frac{1}{2}}^\varepsilon(n,q,p) + \mathcal{O}(\varepsilon)\,.
\end{aligned} \tag{4.17}$$

Hence for $a \in C^\infty(\mathbb{R}^6 \times S^2)$ we define its quantization as acting in the original representation through (3.50) with $\Delta_{\frac{1}{2}}(n)$ replaced by $\Delta_{\frac{1}{2}}^\varepsilon(n,q,p)$. This is consistent, since, using spin-quantization with kernel $\Delta_{\frac{1}{2}}^\varepsilon(n,q,p)$, one has

$$\frac{\hbar\sqrt{3}}{2}\, \widehat{n} = \widehat{S} + \mathcal{O}(\varepsilon^\infty)\,,$$

and the statement of Corollary 4.7 becomes

$$\Big\| \Big(\mathrm{e}^{\mathrm{i}\widehat{H}_{\mathrm{D}}t/(\varepsilon\hbar)}\, \widehat{n}\, \mathrm{e}^{-\mathrm{i}\widehat{H}_{\mathrm{D}}t/(\varepsilon\hbar)} - \widehat{n(t)} \Big) \Pi_+^\varepsilon \Big\| \leq \varepsilon\, C_T\,.$$

In summary we obtain an Egorov theorem based on the skew-product flow Φ_0^t on $\mathbb{R}^6 \times S^2$ also for observables in the original representation.

Theorem 4.9. *Let $a \in C^\infty(\mathbb{R}^6 \times S^2)$ such that $a(\cdot,\cdot,n) \in S^0_1(\mathbb{R})$ for all $n \in S^2$. Then for all $T < \infty$ there is a constant $C_T < \infty$ such that for all $t \in [-T,T]$*

$$\left\| \left(\mathrm{e}^{\mathrm{i}\widehat{H}_{\mathrm{D}} t/(\varepsilon\hbar)}\, \widehat{a}\, \mathrm{e}^{-\mathrm{i}\widehat{H}_{\mathrm{D}} t/(\varepsilon\hbar)} - \widehat{a \circ \Phi_0^t} \right) \Pi_+^\varepsilon \right\| \leq \varepsilon\, C_T\,.$$

4.1.3 Back-reaction of spin onto the translational motion

The semiclassical limit for Dirac electrons yields at leading order a translational dynamics for electrons which is independent of spin. The spin dynamics is given through the T-BMT equation (4.13) resp. (4.15), which is solved along the spin independent trajectories. The goal of this section is to determine the first order corrections to the semiclassical limit of the translational motion and, in particular, to determine its dependence on spin. Physically speaking, one expects the force due to spin to be of the order of the gradient of the magnetic field, i.e. of order ε^2. Since it acts for times of order ε^{-1} the net effect on the trajectories should be of order ε and hence visible in the first order correction to the classical flow.

For pedagogical reasons we briefly discuss how this question can be attacked along the lines of the higher order Egorov theorem in the reference space sketched in Section 3.4.1. While in general one would need $h_{\mathrm{e},2}$ in order to solve the equation (3.43) for the time-evolution of the subprincipal symbol of a semiclassical observable, the semiclassical limit of observables with scalar principal symbol, i.e. of the type $\widehat{b} = \widehat{b}_0 \mathbf{1}_{\mathbb{C}^2} + \mathcal{O}(\varepsilon)$, $b_0 \in S^0_1(\mathbb{R})$, can be determined without this explicit information. For such an observable the principal symbol $b_0(t)$, i.e. the solution to (3.42), will remain scalar and thus its commutator with $h_{\mathrm{e},2}$ in (3.43) vanishes identically for all times. The solution $b_1(t)$ of (3.43) with initial condition $b_1(0) = 0$, is not scalar, in general. Hence, at this order there is back reaction of the spin dynamics on the translational motion. We illustrate this point for the position operator $x(q,p) = x_0(q,p) := q\,\mathbf{1}_{\mathbb{C}^2}$. Then $x_0(q,p,t) = x_0\big(\Phi_+^t(q,p)\big)$ and $x_1(t)$ is obtained, according to Equation (3.43), as the solution of

$$\frac{\mathrm{d}\, x_1(t)}{\mathrm{d}t} = \{E_+ \mathbf{1}, x_1(t)\} + \mathrm{i}[h_{\mathrm{e},1}, x_1(t)] + \{h_{\mathrm{e},1}, x_0(t)\} \tag{4.18}$$

with initial condition $x_1(0) = 0$. The homogeneous part of this equation is just the classical translational and spin motion and the inhomogeneity is

$$\{h_{\mathrm{e},1}, x_0(t)\} = -\frac{\hbar}{2}\, \boldsymbol{\sigma} \cdot \{\, \Omega, x_0(t)\}\,, \tag{4.19}$$

which is not scalar and thus responsible for the splitting of trajectories of electrons with distinct spin orientation. Hence, as in (3.48),

$$x_1(t) = -\frac{\hbar}{2} \int_0^t \mathrm{d}t'\, \mathcal{U}(t-t')\, \boldsymbol{\sigma} \cdot \{\, \Omega,\, x_0(t')\}\,, \tag{4.20}$$

where $\mathcal{U}(t)$ is the "classical flow" defined through (3.47).

Without claim of rigor, we observe in (4.6) that for small velocities $v(q,p)$ one has

$$\Omega(q,p) \approx \frac{e}{mc}\, B(q)\,.$$

Let us further assume that $B(q) = b\, q_z\, e_z$, then

$$\frac{\hbar}{2}\,\boldsymbol{\sigma}\cdot\{\Omega, x_0(t)\} = \frac{\hbar e}{2mc}\boldsymbol{\sigma}_z \frac{\partial B}{\partial q_z}\,\frac{\partial \Phi_q^t}{\partial p_z} = t\,\frac{\hbar e}{2m^2c}\begin{pmatrix} b & 0 \\ 0 & -b \end{pmatrix}$$

and thus according to (4.18), (4.19) the correction to the velocity is proportional to t, corresponding to a constant force with absolute value

$$\hbar e/(2mc)|\nabla B|\,,$$

as expected for a spin-$\frac{1}{2}$ particle.

We conclude this extended remark with reemphasizing that the physically important back-reaction of the fast degrees of freedom, i.e. spin in the present setting, onto the dynamics of the slow degrees of freedom, i.e. the translational motion of the electron, can be seen only in a space-adiabatic expansion, but not in the time-adiabatic approach sketched in Section 1.2.

While the first order correction to the semiclassical dynamics of the position operator in terms of (4.20) contains implicitly all relevant information at this order, its hard to read off any interesting physics from it. In the remainder of the section we argue that a better understanding of the first order corrections to the semiclassical translational dynamics follows from implementing the first order corrections directly in the classical flow Φ_0^t of (4.14) by making it ε-dependent. This seems to be a non-standard strategy and we will discuss the analogous problem for the semiclassics of Bloch electrons in Section 5.3. The second drawback of (4.20) is that it gives the semiclassical evolution of the position operator in the reference representation. This agrees with the position operator of the Dirac equation only at leading order, a fact we used when deriving (4.10) and (4.11). If we are interested in the first order corrections to the dynamics of the true position operator, we need to take into account corrections from the unitary transformation to the reference space.

The main result of this section is Theorem 4.12, an Egorov theorem for observables in the original representation based on ε-dependent classical equations of motion on the phase space $\mathbb{R}^6 \times S^2$, describing a relativistic electron with spin. Readers only interested in the result might jump directly to the paragraph in front of Theorem 4.12 and skip the rather lengthy derivation.

In order to get our hands on the first order corrections to the classical flow Φ_0^t, we once more attack the problem first in the reference representation. Our aim is to find a modified flow $\Phi_\varepsilon^t : \mathbb{R}^6 \times S^2 \to \mathbb{R}^6 \times S^2$ such that (4.16) can be improved to

$$\| \mathrm{e}^{\mathrm{i}\widehat{h}_e t/(\varepsilon\hbar)}\ \widehat{a}\ \mathrm{e}^{-\mathrm{i}\widehat{h}_e t/(\varepsilon\hbar)} - \widehat{a\circ\Phi_\varepsilon^t}\,\| \leq\ \varepsilon^2\, C_T\,. \tag{4.21}$$

To achieve this one has to make sure that the principal symbol $a_0(t)$ and the subprincipal symbol $a_1(t)$ of $a \circ \Phi_\varepsilon^t$ satisfy the equations (3.42) and (3.43). We know already that this is possible without knowing $\widehat{h}_2$, if we restrict ourselves to the case of observables with "spin independent" principal symbol a_0, i.e. $a_0(q,p,n) = a_0(q,p)$ does not depend on $n \in S^2$.

A natural candidate for such a flow Φ_ε^t is the Hamiltonian flow of the symbol of $\widehat{h}_0 + \varepsilon \widehat{h}_1$, i.e. of

$$h^\varepsilon(q,p,n) = E_+(q,p) + \frac{\varepsilon\hbar\sqrt{3}}{2}\, \Omega(q,p) \cdot n \tag{4.22}$$

on $\mathbb{R}^6 \times S^2$. To make this precise, recall that the area two-form on S^2 turns the latter into a symplectic manifold. Properly normalized the corresponding Poisson bracket $\{\cdot,\cdot\}_{S^2}$ for functions on S^2 yields, in particular,

$$\{a \cdot n, n\}_{S^2} = \tfrac{1}{\sqrt{3}}\, a \times n\,.$$

Hence, defining

$$\{\cdot,\cdot\}_{\mathbb{R}^6 \times S^2} := \{\cdot,\cdot\}_{\mathbb{R}^6} + \tfrac{1}{\varepsilon}\{\cdot,\cdot\}_{S^2}\,,$$

the Hamiltonian equations of motion derived from $h^\varepsilon(q,p,n)$ are

$$\begin{aligned}
\dot q &= \{h^\varepsilon, q\}_{\mathbb{R}^6\times S^2} = \{h^\varepsilon, q\}_{\mathbb{R}^6} = \nabla_p\, E_+(q,p) - \frac{\varepsilon\hbar\sqrt{3}}{2}\, \nabla_p\big(n \cdot \Omega(q,p)\big) \\
\dot p &= \{h^\varepsilon, p\}_{\mathbb{R}^6\times S^2} = \{h^\varepsilon, p\}_{\mathbb{R}^6} = -\nabla_q\, E_+(q,p) + \frac{\varepsilon\hbar\sqrt{3}}{2}\, \nabla_q\big(n \cdot \Omega(q,p)\big) \\
\dot n &= \{h^\varepsilon, n\}_{\mathbb{R}^6\times S^2} = \{h^\varepsilon, n\}_{S^2} = n \times \Omega(q,p)\,.
\end{aligned} \tag{4.23}$$

The equations of motion (4.23) define an ε-dependent Hamiltonian flow Φ_ε^t on the phase space $\mathbb{R}^6 \times S^2$. We emphasize that, in contrast to the skew-product flow Φ_0^t, the spin degree of freedom now influences the translational motion.

It is not a completely obvious fact that the ε-dependent flow Φ_ε^t gives rise to an improved Egorov theorem for observables independent of spin.

Proposition 4.10. *Let Φ_ε^t be the solution flow of (4.23) and $a(q,p) \in S_1^0(\mathbb{R}^6)$ a classical observable independent of $n \in S^2$. Then for all $T < \infty$ there is a constant $C_T < \infty$ such that for all $t \in [-T,T]$*

$$\| \, \mathrm{e}^{\mathrm{i}\widehat{h}_{\mathrm{e}} t/(\varepsilon\hbar)}\, \widehat{a}\, \mathrm{e}^{-\mathrm{i}\widehat{h}_{\mathrm{e}} t/(\varepsilon\hbar)} - \widehat{a \circ \Phi_\varepsilon^t} \, \| \le \varepsilon^2\, C_T\,. \tag{4.24}$$

Proof. Let $(Q(q,p,n,t), P(q,p,n,t), N(q,p,n,t))$ be the solution of (4.23) with initial condition (q,p,n). In view of (3.42) and (3.43) we need to show that the matrix-valued symbol corresponding to

$$a(q,p,n,t) := (a \circ \Phi_\varepsilon^t)(q,p,n) := a\big(\, Q(q,p,n,t), P(q,p,n,t)\,\big)\,,$$

which is given through

$$A(q,p,t) := 2\int_{S^2} \mathrm{d}\lambda(n)\, a(q,p,n,t)\, \Delta_{\frac{1}{2}}(n)\,,$$

solves the Moyal-Heisenberg equation

$$\begin{aligned}\partial_t A(t) &= \{h_{\mathrm{e}}, A(t)\} + \mathrm{i}[\, h_{\mathrm{e}},\, A(t)\,] \\ &= \{h_{\mathrm{e}}, A(t)\} - \mathrm{i}\tfrac{\hbar}{2}[\, \boldsymbol{\sigma}\cdot\Omega,\, A(t)\,] \end{aligned} \tag{4.25}$$

up to terms of order ε^2. Recall that this equation obtains its simple form because the principal symbol of $\widehat{a}(t) = \mathrm{e}^{\mathrm{i}\widehat{h}_{\mathrm{e}}t/(\varepsilon\hbar)}\ \widehat{a}\ \mathrm{e}^{-\mathrm{i}\widehat{h}_{\mathrm{e}}t/(\varepsilon\hbar)}$ is a scalar multiple of $\mathbf{1}_{\mathbb{C}^2}$ and remains so under the time evolution. On the other hand it follows from the equations of motion (4.23) that also

$$a\big(\, Q(q,p,n,t), P(q,p,n,t)\,\big) =: a_0(q,p,t) + \varepsilon a_1(q,p,n,t) + \mathcal{O}(\varepsilon^2)$$

has a principal symbol independent of n for all times.

Using these facts we find for the first term on the right hand side of (4.25) that

$$\begin{aligned}\{h_{\mathrm{e}}, A(t)\} &= 4\int_{S^2}\mathrm{d}n\int_{S^2}\mathrm{d}m\,\Big\{E_+ + \varepsilon\sqrt{3}\Omega\cdot m, a_0(t) + \varepsilon a_1(n,t)\Big\}\ \Delta(m)\,\Delta(n) \\ &= 2\int_{S^2}\mathrm{d}n\,\Big\{E_+ + \varepsilon\sqrt{3}\Omega\cdot n, a_0(t) + \varepsilon a_1(n,t)\Big\}\ \Delta(n) + \mathcal{O}(\varepsilon^2) \\ &= 2\int_{S^2}\mathrm{d}n\ \{h^\varepsilon(n), a(n,t)\}_{\mathbb{R}^6}\ \Delta(n) + \mathcal{O}(\varepsilon^2)\,.\end{aligned}$$

For the second term in (4.25) we find

$$\begin{aligned}-\mathrm{i}\tfrac{\hbar}{2}[\, \boldsymbol{\sigma}\cdot\Omega,\, A(t)\,] &= -\mathrm{i}\tfrac{\varepsilon\hbar}{2}\,[\, \boldsymbol{\sigma}\cdot\Omega,\, A_1(t)\,] \\ &= -\mathrm{i}\varepsilon\hbar\int_{S^2}\mathrm{d}n\, a_1(n,t)\,[\,\Omega\cdot\boldsymbol{\sigma},\,\Delta(n)\,] \\ &= -\mathrm{i}\varepsilon\hbar\sqrt{\tfrac{3}{4}}\int_{S^2}\mathrm{d}n\, a_1(n,t)\,[\,\Omega\cdot\boldsymbol{\sigma},\, n\cdot\boldsymbol{\sigma}\,] \\ &= \varepsilon\hbar\sqrt{3}\int_{S^2}\mathrm{d}n\, a_1(n,t)\,(\Omega\times n)\cdot\boldsymbol{\sigma} \\ &= 2\varepsilon\hbar\int_{S^2}\mathrm{d}n\, a_1(n,t)\,(\Omega\times n)\cdot\nabla_n\Delta(n) \\ &= 2\varepsilon\hbar\int_{S^2}\mathrm{d}n\,(\nabla_n a_1(n,t))\cdot(n\times\Omega)\,\Delta(n) \\ &= 2\int_{S^2}\mathrm{d}n\ \varepsilon\,\{h_1^\varepsilon(n), a_1(n,t)\}_{S^2}\ \Delta(n) \\ &= 2\int_{S^2}\mathrm{d}n\ \tfrac{1}{\varepsilon}\ \{h^\varepsilon(n), a(n,t)\}_{S^2}\ \Delta(n)\,.\end{aligned}$$

Here ∇_n denotes the covariant derivative on the sphere S^2 and we used that $\nabla_n \cdot (\Omega \times n) = 0$ for the integration by parts. Since, by construction,

$$\dot{a}(t) = \{h^\varepsilon, a(t)\}_{\mathbb{R}^6} + \tfrac{1}{\varepsilon}\{h^\varepsilon, a(t)\}_{S^2}\,,$$

$A(t)$ indeed solves (4.25) up to terms of order $\mathcal{O}(\varepsilon^2)$. □

While as a mathematical statement this Egorov theorem for a flow on the extended phase space $\mathbb{R}^6 \times S^2$ is clear enough, the correct physical interpretation requires some care. In particular the factor $\sqrt{3}$ appearing in the equations of motion (4.23) looks surprising at first sight. For a better understanding its helpful to shift the focus from the observables to the states. We define the scalar Wigner transform of $\psi \in L^2(\mathbb{R}^3; \mathbb{C}^2)$ as

$$w^\psi(q,p,n) = \operatorname{Tr} W^\psi(q,p)\, \Delta_{\frac{1}{2}}(n)\,,$$

where $W^\psi(q,p)$ is the matrix-valued Wigner transform defined in (3.51). Then we obtain a generalized version of the duality relation between observables and the Wigner transform as

$$\langle \psi, \widehat{a}\,\psi\rangle_{L^2(\mathbb{R}^3,\mathbb{C}^2)} = 2\int_{\mathbb{R}^{2d}} \mathrm{d}q\,\mathrm{d}p \int_{S^2} \mathrm{d}\lambda(n)\, a(q,p,n)\, w^\psi(q,p,n)\,.$$

Hence we can reformulate Proposition 4.10 in the following way.

Corollary 4.11. *Let $\psi(t) = \mathrm{e}^{-\mathrm{i}\widehat{h}_{\mathrm{e}} t/(\varepsilon\hbar)}\psi_0$. Then for each scalar observable $a \in S^0_1(\mathbb{R}^6)$ and all $T < \infty$ there is a constant $C_{T,a} < \infty$ such that for all $\psi_0 \in L^2(\mathbb{R}^3;\mathbb{C}^2)$ and $t \in [-T,T]$*

$$\left| \big\langle \psi(t), \widehat{a}\ \psi(t)\big\rangle - 2\int_{\mathbb{R}^{2d}} \mathrm{d}q\,\mathrm{d}p \int_{S^2} \mathrm{d}\lambda(n)\, a(q,p)\, \big(w^{\psi_0} \circ \Phi_\varepsilon^{-t}\big)(q,p,n) \right| \le C_{T,a}\,\varepsilon^2\,.$$

It is instructive to compute the Wigner transform of a wave function with constant spin. Let $\varphi_{n_0} \in \mathbb{C}^2$ be a normalized eigenspinor of $n_0 \cdot \boldsymbol{\sigma}$ with eigenvalue $+1$ for some $n_0 \in S^2$ and let

$$\psi_{n_0}(x) = \phi(x)\,\varphi_{n_0}\,, \qquad \phi \in L^2(\mathbb{R}^3)\,.$$

Then the Wigner transform of ψ_{n_0} is

$$w^{\psi_{n_0}}(q,p,n) = w^\phi(q,p)\operatorname{Tr}\varphi_{n_0}\,\Delta_{\frac{1}{2}}(n) = w^\phi(q,p)\,\big(\tfrac{1}{2} + \sqrt{\tfrac{3}{4}}\, n_0 \cdot n\big)\,.$$

Hence even with a wave function ψ_{n_0} having constant spin there is associated a density $w^{\psi_{n_0}}(q,p,n)$ which is smeared out all over the sphere S^2 and, in particular, negative near the antipode of n_0. Note that for such a state the equations of motion (4.23) can be simplified. First of all observe that the evolved Wigner transform will have the form

$$\big(w^{\psi_{n_0}} \circ \Phi_\varepsilon^{-t}\big)(q,p,n) = f(q,p,t)\,\big(\tfrac{1}{2} + \sqrt{\tfrac{3}{4}}\, n_0(q,p,t)\cdot n\big) + \mathcal{O}(\varepsilon)\,,$$

where $n_0(q,p,t)$ solves the T-BMT equation

$$\dot{n}_0 = n_0 \times \Omega(\Phi_+^t(q,p)) \tag{4.26}$$

with initial condition $n_0(q,p,0) \equiv n_0$. Reinserting this into the terms of order ε in (4.23) and integrating out n, we find that, up to errors of order ε^2,

$$\begin{aligned} \dot{q} &= \nabla_p E_+(q,p) - \frac{\varepsilon\hbar}{2}\nabla_p\big(n_0(q,p,t)\cdot\Omega(q,p)\big) \\ \dot{p} &= -\nabla_q E_+(q,p) + \frac{\varepsilon\hbar}{2}\nabla_q\big(n_0(q,p,t)\cdot\Omega(q,p)\big)\,. \end{aligned} \tag{4.27}$$

Hence for states with constant spin the corrections to the classical equations of motion have exactly the size as expected from the corrections to the quantum mechanical Hamiltonian. In particular, the factor $\sqrt{3}$ in (4.23) just compensates for the fact that with a spinor φ_{n_0} there is associated a density $\frac{1}{2} + \sqrt{3/4}\, n_0 \cdot n$ on S^2.

After these remarks on the interpretation of the extended phase space $\mathbb{R}^6 \times S^2$ we turn back to the original question. As explained above, the ε-dependent equations of motion (4.23) are only the first step towards higher order semiclassical equations of motion for a relativistic electron. This is because q and p are the canonical variables in the reference representation. What we are interested in are the equations for position and momentum in the original representation projected onto the almost invariant subspace. While at leading order we could ignore this difference, at subleading order it becomes relevant. According to (3.57) we have that

$$\begin{aligned} Q(q,p) &:= \operatorname{Symb} U^\varepsilon\, \Pi_+^\varepsilon\, \widehat{Q}_{\mathbb{C}^4}\, \Pi_+^\varepsilon\, U^{\varepsilon\,*} = q\,\mathbf{1}_{\mathbb{C}^2} + \varepsilon \boldsymbol{\mathcal{A}}\big(p - \tfrac{e}{c}A(q)\big) + \mathcal{O}(\varepsilon^2) \\ P(q,p) &:= \operatorname{Symb} U^\varepsilon\, \Pi_+^\varepsilon\, \widehat{P}_{\mathbb{C}^4}\, \Pi_+^\varepsilon\, U^{\varepsilon\,*} = \\ &= p\,\mathbf{1}_{\mathbb{C}^2} + \varepsilon\frac{e}{c}\sum_{j=1}^{3} \boldsymbol{\mathcal{A}}_j\big(p - \tfrac{e}{c}A(q)\big)\,\nabla_q A_j(q) + \mathcal{O}(\varepsilon^2)\,, \end{aligned}$$

where

$$\boldsymbol{\mathcal{A}}(\pi) = -\frac{\hbar c^2}{2E_0(\pi)(E_0(\pi)+mc^2)}\;\boldsymbol{\sigma}\times\pi$$

is the coefficient of the Berry connection introduced in Remark 4.3. The scalar symbols on the extended phase space are thus

$$\begin{aligned} Q(q,p,n) &= q \;\; + \varepsilon \mathcal{A}\big(p - \tfrac{e}{c}A(q), n\big) + \mathcal{O}(\varepsilon^2) \\ P(q,p,n) &= p + \varepsilon\frac{e}{c}\sum_{j=1}^{3} \mathcal{A}_j\big(p - \tfrac{e}{c}A(q), n\big)\,\nabla_q A_j(q) + \mathcal{O}(\varepsilon^2)\,, \end{aligned}$$

with

$$\mathcal{A}(\pi, n) = -\frac{\hbar c^2 \sqrt{3}}{2E_0(\pi)(E_0(\pi) + mc^2)}\, n \times \pi\,.$$

In order to obtain the desired equations of motion for Q and P, we just have to make the change of variables $q \mapsto q(Q, P, n)$ and $p \mapsto p(Q, P, n)$ in the equations of motion (4.23), where we may drop all terms of order ε^2. The computation and the result become simpler, if we work with the kinetic momenta instead of the canonical momenta. Let

$$\pi = p - \tfrac{e}{c}\, A(q) \quad \text{and} \quad \Pi = P - \tfrac{e}{c}\, A(Q)\,,$$

then one finds

$$Q(q, \pi, n) = q + \varepsilon\, \mathcal{A}(\pi, n) \quad \text{and} \quad \Pi(q, \pi, n) = \pi + \varepsilon\, \tfrac{e}{c}\, \mathcal{A}(\pi, n) \times B(q)\,.$$

The inverse transformation is

$$q(Q, \Pi, n) = Q\ - \varepsilon\, \mathcal{A}(\Pi, n) \quad \text{and} \quad \pi(Q, \Pi, n) = \Pi - \varepsilon\, \tfrac{e}{c}\, \mathcal{A}(\Pi, n) \times B(Q)\,, \tag{4.28}$$

again only up to terms of order ε^2. Using

$$h_{\mathrm{e},1}(q, \pi, n) = -M(\pi, n) \cdot B(q) - e\, \mathcal{A}(\pi, n) \cdot E(q)$$

with

$$M(\pi) = \frac{\hbar e c \sqrt{3}}{2E_0(\pi)}\, n\,,$$

as introduced in Remark 4.3, the canonical equations of motion (4.23) for q and p read in the new variables

$$\begin{aligned} \dot{q} &= \nabla E_0(\pi) - \varepsilon\, \nabla_\pi \big(M(\pi, n) \cdot B(q) + e\, \mathcal{A}(\pi, n) \cdot E(q) \big) \\ \dot{\pi} &= eE(q) + \tfrac{e}{c}\, \dot{q} \times B(q) + \varepsilon\, \nabla_q \big(M(\pi, n) \cdot B(q) + e\, \mathcal{A}(\pi, n) \cdot E(q) \big)\,. \end{aligned} \tag{4.29}$$

We now make the substitution $q \mapsto q(Q, \Pi, n)$ and $\pi \mapsto \pi(Q, \Pi, n)$ in (4.29) and drop all terms of order ε^2 without further notice. In order to assure readability, we use the convention that summation over indices appearing twice is implicit and we abbreviate $\partial_j f = f_{,j}$. For $\dot{Q}$ we find, using Taylor expansion,

$$\begin{aligned} \dot{Q}_j &= \dot{q}_j + \varepsilon\, \mathcal{A}_{j,l} \dot{\pi}_l \\ &= E_{0,j} - \varepsilon\, \tfrac{e}{c} E_{0,jl}\, (\mathcal{A} \times B)_l - \varepsilon\, M_{l,j} B_l - \varepsilon\, e \mathcal{A}_{l,j} E_l \\ &\quad + \varepsilon\, e \mathcal{A}_{j,l} E_l + \varepsilon\, \tfrac{e}{c} \mathcal{A}_{j,l} (\nabla E_0 \times B)_l \\ &= E_{0,j} - \varepsilon\, \tfrac{e}{c} E_{0,jl}\, (\mathcal{A} \times B)_l - \varepsilon\, M_{l,j} B_l \\ &\quad + \varepsilon\, e E_l (\mathcal{A}_{j,l} - \mathcal{A}_{l,j}) + \varepsilon\, \tfrac{e}{c} \mathcal{A}_{j,l} (\nabla E_0 \times B)_l\,. \end{aligned}$$

In order to simplify this expression we introduce the curvature of the Berry connection

$$\Omega_{\mathcal{A}} := \nabla \times \mathcal{A} = \frac{\hbar c^2 \sqrt{3}\,\big(2 - \frac{1}{1+\gamma}\big)}{2E_0(E_0 + mc^2)}\,\beta \times (n \times \beta) \tag{4.30}$$

and write for the leading order velocity $v(\Pi) = \nabla E_0(\Pi) = c^2\Pi/E_0(\Pi)$ and and abbreviate also $\beta(\Pi) = v(\Pi)/c$. Then

$$\begin{aligned}\dot{Q} &= v + \varepsilon\, eE \times \Omega_{\mathcal{A}} \\ &\quad + \varepsilon\, \frac{\hbar e c^2 \sqrt{3}}{2E_0(E_0 + mc^2)} \Big[\beta \times (B \times n) + \beta \Big((1 + \tfrac{1}{\gamma})\,(n \cdot B) - (\beta \times B) \cdot (\beta \times n) \Big) \Big]\,.\end{aligned} \tag{4.31}$$

We now turn to the equation of motion for Π. Substituting $q \mapsto q(Q, \Pi, n)$ and $\pi \mapsto \pi(Q, \Pi, n)$ in (4.29) gives

$$\begin{aligned}\dot{\Pi}_j &= \dot{\pi}_j + \varepsilon\, \tfrac{e}{c} \tfrac{\mathrm{d}}{\mathrm{d}t} (\mathcal{A} \times B) \\ &= eE_j - \varepsilon\, eE_{j,l}\mathcal{A}_l + \tfrac{e}{c}(\dot{Q} \times B)_j - \varepsilon\, \tfrac{e}{c}(\dot{\mathcal{A}} \times B)_j - \varepsilon\, \tfrac{e}{c}\big(\dot{Q} \times ((\mathcal{A} \cdot \nabla)B)\big)\big)_j \\ &\quad + \varepsilon\, e\mathcal{A}_l E_{l,j} + \varepsilon\, B_{l,j} M_l + \varepsilon\, \tfrac{e}{c}(\dot{\mathcal{A}} \times B)_j + \varepsilon\, \tfrac{e}{c}\big(\mathcal{A} \times ((\dot{Q} \cdot \nabla)B)\big)_j \\ &= eE_j + \tfrac{e}{c}(\dot{Q} \times B)_j + \varepsilon\, B_{l,j} M_l - \varepsilon\, \tfrac{e}{c}\mathcal{A}_l (\dot{Q} \times B)_{l,j}\,.\end{aligned}$$

Evaluating the last expression, we finally obtain

$$\dot{\Pi} = eE + \tfrac{e}{c}\dot{Q} \times B + \varepsilon\, \frac{\hbar e m c^3 \sqrt{3}}{2E_0^2} \nabla(n \cdot B) + \varepsilon\, \frac{\hbar e c \sqrt{3}}{2(E_0 + mc^2)}\,(\beta \cdot n)\,\nabla(\beta \cdot B)\,. \tag{4.32}$$

The formal derivation of the equations of motion (4.31) and (4.32) starting from the flow (4.23) and the corresponding Egorov theorem, Proposition 4.10, can easily be turned into a rigorous result, which we now state in a theorem. We omit the details of the argument, which are exactly analogous to parts of the proof of Theorem 5.2 in Section 5.3.

For sake of better readability we change notation back from (Q, Π) to (q, π). The purpose of the capital letters was only to clearly distinguish the physical semiclassical observables (Q, Π) from the coordinates (q, π) in the reference representation. Let

$$\Phi_\varepsilon^t : \mathbb{R}^6 \times S^2 \to \mathbb{R}^6 \times S^2, \quad (q, \pi, n) \mapsto (q(t), \pi(t), n(t))\,,$$

be the solution flow of

$$\begin{aligned}\dot{q} &= v + \varepsilon\, eE \times \Omega_{\mathcal{A}} \\ &\quad + \varepsilon\, \frac{\hbar e c^2 \sqrt{3}}{2E_0(E_0 + mc^2)} \Big[\beta \times (B \times n) + \beta \Big((1 + \tfrac{1}{\gamma})\,(n \cdot B) - (\beta \times B) \cdot (\beta \times n) \Big) \Big]\end{aligned}$$

$$\dot{\pi} = eE + \tfrac{e}{c}\dot{q} \times B + \varepsilon\, \frac{\hbar e m c^3 \sqrt{3}}{2E_0^2} \nabla(n \cdot B) + \varepsilon\, \frac{\hbar e c \sqrt{3}}{2(E_0 + mc^2)}\,(\beta \cdot n)\,\nabla(\beta \cdot B)$$

$$\dot{n} = n \times \Omega(q, \pi)\,,$$

where we recall that $B(q)$ is the magnetic field, $E(q)$ the electric field, $E_0(\pi) = c\sqrt{m^2c^2 + \pi^2}$ the relativistic kinetic energy, $v(\pi) = c^2\pi/E_0(\pi)$ the velocity, $\beta(\pi) = v(\pi)/c$ and $\gamma(\pi) = E_0(\pi)/(mc^2)$. The curvature $\Omega_{\mathcal{A}}(\pi)$ of the Berry connection $\mathcal{A}(\pi)$ is defined in (4.30).

For comparison with the quantum dynamics we need to switch back to the canonical variables and denote the corresponding flow as

$$\overline{\Phi}^t_\varepsilon(q,p,n) := \begin{pmatrix} \Phi^t_{\varepsilon\, q}\big(q, p - \frac{e}{c}A(q), n\big) \\ \Phi^t_{\varepsilon\, \pi}\big(q, p - \frac{e}{c}A(q), n\big) + \frac{e}{c}A(q) \\ \Phi^t_{\varepsilon\, n}\big(q, p - \frac{e}{c}A(q), n\big) \end{pmatrix}.$$

Then for scalar observables Theorem 4.9 can be improved.

Theorem 4.12. *Let $a \in S^0_1(\mathbb{R})$. Then for all $T < \infty$ there is a constant $C_T < \infty$ such that for all $t \in [-T, T]$*

$$\Big\| \Pi^\varepsilon_+ \Big(\mathrm{e}^{\mathrm{i}\widehat{H}_{\mathrm{D}} t/(\varepsilon\hbar)}\, \widehat{a}\, \mathrm{e}^{-\mathrm{i}\widehat{H}_{\mathrm{D}} t/(\varepsilon\hbar)} - \widehat{a \circ \overline{\Phi}^t_\varepsilon} \Big) \Pi^\varepsilon_+ \Big\| \leq \varepsilon^2\, C_T\,,$$

where $a \circ \overline{\Phi}^t_\varepsilon(q,p,n) := a\big(\Phi^t_{\varepsilon\, q}(q,p,n), \Phi^t_{\varepsilon\, p}(q,p,n)\big)$.

Remark 4.13. For the reader who skipped the derivation, we recall that with the scalar symbol $a \circ \overline{\Phi}^t_\varepsilon$ depending on $n \in S^2$ we associate a $\mathcal{L}(\mathbb{C}^4)$-valued symbol $A \circ \overline{\Phi}^t_\varepsilon$ through

$$(A \circ \overline{\Phi}^t_\varepsilon)(q,p) = 2 \int_{S^2} \mathrm{d}\lambda(n)\, (a \circ \overline{\Phi}^t_\varepsilon)(q,p,n)\, \widetilde{\Delta}_{\frac{1}{2}}(n,q,p)\,,$$

where $\widetilde{\Delta}_{\frac{1}{2}}(n,q,p)$ was defined in (4.17). Hence $\widehat{a \circ \overline{\Phi}^t_\varepsilon}$ in the statement of Theorem 4.12 is understood to be the usual Weyl quantization of $A \circ \overline{\Phi}^t_\varepsilon$.

Furthermore note that for initial states in $\mathrm{Ran}\Pi^\varepsilon_+$ with constant spin, i.e. states satisfying

$$n_0 \cdot \widehat{S}\, \Psi_0 = \Psi_0 + \mathcal{O}(\varepsilon^2)$$

for some $n_0 \in S^2$, the classical equations of motion simplify to

$$\begin{aligned} \dot{q} &= v + \varepsilon\, eE \times \Omega_{\mathcal{A}}(n_0(t)) + \varepsilon\, \frac{\hbar e c^2}{2E_0(E_0 + mc^2)} \Big[\beta \times (B \times n_0(t)) \\ &\qquad + \beta \Big((1 + \tfrac{1}{\gamma})\, (n_0(t) \cdot B) - (\beta \times B) \cdot (\beta \times n_0(t)) \Big) \Big] \\ \dot{\pi} &= eE + \tfrac{e}{c}\dot{q} \times B + \varepsilon\, \frac{\hbar e m c^3}{2E_0^2} \nabla (n_0(t) \cdot B) \\ &\qquad + \varepsilon\, \frac{\hbar e c}{2(E_0 + mc^2)}\, (\beta \cdot n_0(t))\, \nabla (\beta \cdot B)\,, \end{aligned}$$

where $n_0(t)$ is the solution of the T-BMT equation (4.26). This follows by the same argument which led to (4.27). The latter showed, in particular,

that the factor $\sqrt{3}$ appearing in the classical equations (4.31) and (4.32) just compensates for the fact that with a spinor φ_{n_0} there is associated a density $\frac{1}{2} + \sqrt{3/4}\, n_0 \cdot n$ on S^2. ♢

Remark 4.14. In the classical limit to leading order all dependence on the "slow variation parameter" ε disappears. However, when one wants to solve the classical equations of motion (4.31) and (4.32) in a concrete application, i.e. for explicitly given external fields, one now faces the problem to read off a value for ε. As to be discussed in Section 4.4, the solution to this problem is to set $\varepsilon = 1$ in the final effective equations. More precisely, the equations of motion (4.31) and (4.32) without ε describe the approximate semiclassical behavior of a Dirac electron for sufficiently weak and smooth external fields. ♢

4.2 Time-dependent Born-Oppenheimer theory: Part II

We now come back to the paradigmatic system of adiabatic theory, namely to Born-Oppenheimer type Hamiltonians, cf. (2.29), of the form

$$H_{\mathrm{BO}}(q,p) = \frac{1}{2}\big(p - \varepsilon A(q)\big)^2 \mathbf{1}_{\mathcal{H}_{\mathrm{f}}} + H_{\mathrm{e}}(q)\,. \tag{4.33}$$

Recall that $H_{\mathrm{e}}(q)$ is the electronic Hamiltonian for fixed nuclear configuration $q \in \mathbb{R}^d$ with an electronic energy band $e_{\mathrm{r}}(q)$ of constant multiplicity ℓ, i.e. $H_{\mathrm{e}}(q)\pi_0(q) = e_{\mathrm{r}}(q)\pi_0(q)$. To simplify the discussion we assume that $H_{\mathrm{e}} \in S^0(\mathcal{L}(\mathcal{H}_{\mathrm{f}}))$ and for the magnetic potential $A(q)$ that $A \in C^\infty_{\mathrm{b}}(\mathbb{R}^d, \mathbb{R}^d)$. For Born-Oppenheimer type Hamiltonians adiabatic decoupling in the spirit of Chapter 3 is established with exponentially small errors by Martinez and Sordoni [MaSo], see also [So]. However, in [MaSo, So] no attempt was made to compute and analyze the effective Hamiltonian beyond leading order.

Note that the quadratic growth of $H_{\mathrm{BO}\,0}(q,p) = \frac{1}{2}p^2 + H_{\mathrm{e}}(q)$ as a function of p prevents us from applying the general results of Chapter 3 directly. As to be discussed below, energy cutoffs need to be introduced. For the moment we ignore this problem and proceed by working out the perturbative scheme for computing the effective Hamiltonian formally.

We fix arbitrarily an orthonormal basis $\{\psi_\alpha(q)\}_{\alpha=1}^{\ell}$ of $\mathrm{Ran}\pi_0(q)$ depending smoothly on q, which then satisfies $H_{\mathrm{BO}\,0}(q,p)\psi_\alpha(q) = E_{\mathrm{r}}(q,p)\psi_\alpha(q)$ with $E_{\mathrm{r}}(q,p) = \frac{1}{2}p^2 + e_{\mathrm{r}}(q)$ for $1 \le \alpha \le \ell$. Only the first and second term of formula (3.40) contributes and yields

$$h_{1\,\alpha\beta}(q,p) = -p \cdot A(q) - \mathrm{i}\, p \cdot \langle \psi_\alpha(q), \nabla_q \psi_\beta(q)\rangle =: -p \cdot A(q) - p \cdot \mathcal{A}_{\alpha\beta}(q)\,,$$

which is well known in the case of a nondegenerate eigenvalue, [ShWi, LiWe$_1$], and agrees with (2.46) in Section 2.3. $\mathcal{A}_{\alpha\beta}(q)$ has the geometrical meaning of a gauge potential, i.e. coefficients of a connection on the trivial bundle $\mathbb{R}^d \times \mathbb{C}^\ell$, the Berry connection, cf. Section 2.3.4 and Section 3.4.2.

For the Born-Oppenheimer Hamiltonian the calculation of $h_{2\,\alpha\beta}$ is still feasible without much effort and the result is

$$h_{2\,\alpha\beta} = \frac{1}{2}|A(q)|^2 + \frac{1}{2}\sum_{\mu=1}^{\ell} \mathcal{A}_{\alpha\mu}\cdot\mathcal{A}_{\mu\beta} \tag{4.34}$$
$$+\frac{1}{2}\langle\nabla_q\psi_\alpha, (1-\pi_0)\cdot\nabla_q\psi_\beta\rangle - \langle\, p\cdot\nabla_q\psi_\alpha, R_0(E_{\rm r})\; p\cdot\nabla_q\psi_\beta\rangle\,.$$

Recall the definition of $R_0(E_{\rm r}) = (H_{{\rm BO}\,0} - E_{\rm r})^{-1}(1-\pi_0)$, which reduces to $R_0(E_{\rm r})(q) = (H_{\rm e}(q) - e_{\rm r}(q))^{-1}(1-\pi_0(q))$ in the present case. Although we omit the details of the computation leading to (4.34), we shortly describe how (3.37) relates to (4.34).

Clearly the first term in (3.37) produces the first term (4.34). Since u_0 and π_0 are functions of q only, the second term in (3.38) is the only one contributing to u_1, and thus the second and the third term in (3.37) vanish after projecting with the $\pi_{\rm r}$'s from outside the brackets. The last two terms in (3.37) cancel each other. The seventh term in (3.37) yields the second term in (4.34) and the fourth and sixth term in (3.37) combine to the third and the fourth term in (4.34). In particular the calculation yields for the symbol of the unitary

$$u^*_{\rm BO}(q,p)\pi_{\rm r} = \sum_{\alpha=1}^{\ell}\Big(|\psi_\alpha(q)\rangle + {\rm i}\varepsilon\, R_0(E_{\rm r})(q)\;|\,p\cdot\nabla_q\psi_\alpha(q)\rangle\Big)\langle\chi_\alpha| + \mathcal{O}(\varepsilon^2)\,.$$

Thus the symbol of the second order effective Born-Oppenheimer Hamiltonian reads

$$\begin{aligned} h_{{\rm BO}\,\alpha\beta}(q,p) = {}& \frac{1}{2}\Big(p - \varepsilon\, A(q) - \varepsilon\,\mathcal{A}(q)\Big)^2_{\alpha\beta} + \; e_{\rm r}(q)\delta_{\alpha\beta} \\ & + \frac{\varepsilon^2}{2}\langle\nabla_q\psi_\alpha(q), (1-\pi_0(q))\cdot\nabla_q\psi_\beta(q)\rangle \\ & - \varepsilon^2\,\langle\, p\cdot\nabla_q\psi_\alpha(q),\; R_0(E_{\rm r})(q)\; p\cdot\nabla_q\psi_\beta(q)\rangle + \mathcal{O}(\varepsilon^3)\,, \end{aligned} \tag{4.35}$$

where the first two terms from (4.34) nicely complete the square in the first term in (4.35). Note that the third term on the right side of (4.35) depends on q only and was interpreted in [Be$_3$] as a geometric electric potential in analogy to the geometric vector potential $\mathcal{A}(q)$. For a further discussion of the role of the different terms in (4.35) within an explicit example we refer to Section 4.5.

In the special case of a nondegenerate eigenvalue $e_{\rm r}$ and a matrix-valued Hamiltonian H without magnetic potential, (4.35) reduces to the expression obtained by Littlejohn and Weigert [LiWe$_1$]. They also remark that the previous studies [ShWi, AhSt] of the expansion of the effective Born-Oppenheimer Hamiltonian missed the last term in (4.35). Indeed, e.g. in [Be$_3$] the second order contributions to the effective Hamiltonian were computed from expanding

$$\tilde{H}_{\text{eff}} = \widehat{\pi}_0 \, \widehat{H}_{\text{BO}} \, \widehat{\pi}_0$$

to second order in ε, which yields (4.35) without the last term. This is, however, not the correct second order effective Hamiltonian associated with the eigenvalue band $e_{\text{r}}(q)$, since $\text{Ran}\widehat{\pi}_0$ approximates the corresponding almost invariant subspace only to leading order.

The Born-Oppenheimer type Hamiltonians as well as many other physically relevant Hamiltonians do not satisfy the general assumptions we imposed in Chapter 3. This is so for two reasons. First of all they are quantizations of symbols taking values in the unbounded operators. Secondly, the gap does not increase as fast as the Hamiltonian for large momenta, e.g. quadratically in the Born-Oppenheimer setting. The first problem is purely technical and the domain questions which arise have to be dealt with case by case, cf. Chapter 5. The second problem causes a qualitative change in the sense that the adiabatic decoupling is no longer uniform, as can be seen from the construction of the almost invariant subspace in Section 3.1. To deal with the second problem one therefore needs a cutoff for large momenta. There are basically two ways to implement such a cutoff. One possibility is to directly cut off large momenta as was done in Chapter 2, see also [TeSp, SpTe], but then one needs to control the times for which no momenta exceeding the cutoff are produced under the dynamics. However, for a large class of Hamiltonians including the Born-Oppenheimer type Hamiltonian (4.33), cutting off high energies is equivalent to cutting high momenta. Then conservation of energy immediately ensures that no momenta exceeding the cutoff are produced over time. This idea was developed in [So] and also used in [MaSo]. We will briefly indicate an alternative way on how to implement such an energy cutoff in order to fit the Born-Oppenheimer and similar settings into our general assumptions.

Let $H_0 \in S^m_0$ be elliptic and positive, i.e. there is a constant $C > 0$ such that $H_0(q,p) \geq C \langle p \rangle^m$. For example the Born-Oppenheimer Hamiltonian as defined in (4.33) satisfies $H_0 \in S^2_0$ and it is elliptic provided that H_{e} is positive (otherwise just add a constant to H_0 since $H_{\text{e}} \in S^0$). Then we can prove adiabatic decoupling uniformly for energies below any $\lambda \in \mathbb{R}$, i.e. on $\mathbf{1}_{(-\infty,\lambda]}(\widehat{H}_0)\mathcal{H}$.

To see this let $\Lambda = \{(q,p) : H_0(q,p) < \lambda\}$, then bounding the total energy by λ essentially corresponds to confining the slow degrees of freedom to the region Λ in phase space. More precisely, let $\chi_\lambda \in C^\infty_0(\mathbb{R})$ such that $\chi_\lambda|_{[0,\lambda]} = 1$ and $\chi_\lambda|_{[\lambda+\delta,\infty)} = 0$ for some $\delta > 0$, then $\chi_\lambda(\widehat{H}_0) \in \text{OP}S^{-\infty}_0$ is a semiclassical operator. Furthermore, its symbol $\chi := \text{Symb}(\chi_\lambda(\widehat{H}_0))$ has an asymptotic expansion which is identically equal to 1 on Λ, i.e. $\chi|_\Lambda \asymp 1$ and identically equal to 0 on the set where $H_0(q,p) \geq \lambda + \delta$. The statements about $\chi_\lambda(\widehat{H}_0)$ and its symbol follow from the functional calculus for semiclassical operators as developed in [DiSj], Theorem 8.7.

Next we assume that one can define an auxiliary Hamiltonian $H_{\text{aux}}(q,p) \in S^0_0$ such that

(i) $H_{\rm aux}(q,p) = H_0(q,p)$ for all $(q,p) \in \Lambda + \delta := \{(q,p) : H_0(q,p) < \lambda + \delta\}$,
(ii) $H_{\rm aux}(q,p) > H_0(q',p')$ for all $(q,p) \notin \Lambda + \delta$ and $(q',p') \in \Lambda + \delta$
(iii) and $H_{\rm aux}(q,p)$ satisfies the global gap condition $\mathbf{(Gap)}_0$.

This can be easily achieved e.g. in the Born-Oppenheimer setting by replacing p^2 by an appropriate bounded function which flattens at high momenta.

It follows from the previous discussion that $(\widehat{H}_0 - \widehat{H}_{\rm aux})\,\chi_\lambda(\widehat{H}_0) = \mathcal{O}_{-\infty}(\varepsilon^\infty)$ and that $\chi_\lambda(\widehat{H}_0) - \chi_\lambda(\widehat{H}_{\rm aux}) = \mathcal{O}_{-\infty}(\varepsilon^\infty)$.

Using $\chi_\lambda(\widehat{H}_0)\mathbf{1}_{(-\infty,\lambda]}(\widehat{H}_0) = \mathbf{1}_{(-\infty,\lambda]}(\widehat{H}_0)$, one finds, in particular, that

$$\Big(\widehat{H}_0 - \widehat{H}_{\rm aux}\Big)\,\mathbf{1}_{(-\infty,\lambda]}(\widehat{H}_0) = \mathcal{O}_0(\varepsilon^\infty) \tag{4.36}$$

in the norm of bounded operators and thus also

$$\begin{aligned}&\Big(\mathrm{e}^{-\mathrm{i}\widehat{H}_{\rm aux}s} - \mathrm{e}^{-\mathrm{i}\widehat{H}_0 s}\Big)\,\mathbf{1}_{(-\infty,\lambda]}(\widehat{H}_0) \qquad (4.37)\\ &= -\,\mathrm{i}\mathrm{e}^{-\mathrm{i}\widehat{H}_{\rm aux}s}\int_0^s \mathrm{d}s'\,\mathrm{e}^{\mathrm{i}\widehat{H}_{\rm aux}s'}\Big(\widehat{H}_{\rm aux} - \widehat{H}_0\Big)\mathrm{e}^{-\mathrm{i}\widehat{H}_0 s'}\,\mathbf{1}_{(-\infty,\lambda]}(\widehat{H}_0) = \mathcal{O}_0(\varepsilon^\infty|s|)\,.\end{aligned}$$

Now the scheme of Chapter 3 can be applied to $H_{\rm aux}$ and by virtue of (4.36) and (4.37) all results are valid for H_0 up to $\mathcal{O}(\varepsilon^\infty)$ if one restricts to energies below λ. In particular one finds that for $(q,p) \in \Lambda$ the leading order symbols of $h_{\rm aux} = U^\varepsilon \widehat{H}_{\rm aux} U^{\varepsilon\,*}$ are given by the formulas obtained in Section 3.3 using the symbol $H_0(q,p)$.

4.3 The time-adiabatic theorem revisited

With little additional effort adiabatic perturbation theory can be applied even to the time-adiabatic setting, cf. Section 2.1. For the convenience of the reader we recall the basic setup. Given a Hilbert space $\mathcal{H}$ and a family $H^\varepsilon(t)$, $t \in \mathbb{R}$, of self-adjoint operators such that $H^\varepsilon(t) =: H(t,\eta,\varepsilon) \in S^0(\varepsilon, \mathcal{L}(\mathcal{H}))$, the solutions of the equations

$$\mathrm{i}\varepsilon\partial_t U^\varepsilon(t,t') = H^\varepsilon(t)U^\varepsilon(t,t')\,, \qquad t' \in \mathbb{R}\,, \tag{4.38}$$

define a unitary propagator, cf. Definition 1.1. Hence we replace the phase space $\mathbb{R}^d_q \times \mathbb{R}^d_p$ by $\mathbb{R}_t \times \mathbb{R}_\eta$ in the following. It is assumed again that $H_0(t)$, the principal symbol of $H^\varepsilon(t)$, has a relevant part $\sigma_{\rm r}(t)$ of its spectrum, which is separated by a gap from the remainder uniformly for $t \in \mathbb{R}$. As before we denote the spectral projection on $\sigma_{\rm r}(t)$ by $\pi_0(t)$.

The following theorem is a variant of the time-adiabatic theorem of quantum mechanics with higher order estimates, cf. [ASY_1, Ga, JoPf_1, Nen_4], formulated in the language of adiabatic perturbation theory. Sjöstrand first recognized the usefulness of pseudodifferential calculus in this context [Sj].

The proof below can be adapted to the case of a time-dependent operator-valued classical symbol $H(q,p,t)$, as – for example – the Dirac Hamiltonian or the Bloch electron with slowly varying time-dependent external potentials, see Remark 4.16 below.

Theorem 4.15 (Time-adiabatic theorem). *Let $H(t)$ and $\sigma_{\rm r}(t)$ be as above.*

(i) **Decoupled subspace.** *There exists a family of orthogonal projectors $\Pi^\varepsilon(t)$ such that $\Pi^\varepsilon(\cdot) \in S^0(\varepsilon, \mathcal{L}(\mathcal{H}))$, $\Pi^\varepsilon(t) - \pi_0(t) = \mathcal{O}_0(\varepsilon)$ and*

$$U(t,t')^*\,\Pi^\varepsilon(t)\,U(t,t') = \Pi^\varepsilon(t') + \mathcal{O}_0(\varepsilon^\infty|t-t'|) \tag{4.39}$$

uniformly for $t', t \in \mathbb{R}$. Whenever $\partial_t^\alpha H(t) = 0$ for some $t \in \mathbb{R}$ and all $\alpha \in \mathbb{N}$, then $\Pi^\varepsilon(t) = \pi_0(t)$.

(ii) **Intertwining unitaries.** *There exists a family of unitary operators $u_0(\cdot) \in C_{\rm b}^\infty(\mathbb{R}, \mathcal{L}(\mathcal{H}))$ with $u_0(t)\,\pi_0(t)\,u_0^*(t) = \pi_0(0) =: \pi_{\rm r}$ and a family of unitaries $\mathcal{U}^\varepsilon(\cdot) \in S^0(\varepsilon, \mathcal{L}(\mathcal{H}))$ such that*

$$\mathcal{U}^\varepsilon(t)\,\Pi^\varepsilon(t)\,\mathcal{U}^{\varepsilon\,*}(t) = \pi_{\rm r} \quad \textit{and} \quad \mathcal{U}^\varepsilon(t) - u_0(t) = \mathcal{O}_0(\varepsilon)\,.$$

(iii) **Effective dynamics.** *There exists a family of self-adjoint operators $h(t)$, $h(\cdot) \in S^0(\varepsilon, \mathcal{L}(\mathcal{H}))$, such that*

$$[\,h(t),\,\pi_{\rm r}\,] = 0 \qquad \textit{for all} \qquad t \in \mathbb{R}$$

and the solution of the initial value problem

$$\mathrm{i}\varepsilon\partial_t U_{\rm eff}(t,t') = h(t) U_{\rm eff}(t,t')\,, \qquad t' \in \mathbb{R}\,, \qquad U_{\rm eff}(t,t) = \mathbf{1}_{\mathcal{H}}$$

satisfies

$$U(t,t') = \mathcal{U}^{\varepsilon\,*}(t)\,U_{\rm eff}(t,t')\,\mathcal{U}^\varepsilon(t') + \mathcal{O}_0(\varepsilon^\infty|t-t'|)\,. \tag{4.40}$$

The asymptotic expansion of $h(t)$ in $\mathcal{L}(\mathcal{H})$ reads

$$h(t) \asymp \sum_{n=0}^\infty \varepsilon^n \left(\sum_{j+k+l=n} u_j(t)\,H_k(t)\,u_l^*(t) \right.$$
$$\left. +\ \frac{\mathrm{i}}{2} \sum_{j+k+1=n} (u_j(t)\,\dot{u}_k^*(t) - \dot{u}_j(t)\,u_k^*(t)) \right)\,, \tag{4.41}$$

where $\sum_n \varepsilon^n H_n(t)$ is the asymptotic expansion of $H(t)$ in $\mathcal{L}(\mathcal{H})$ and $\sum_n \varepsilon^n u_n$ is the asymptotic expansion of $\mathcal{U}^\varepsilon(t)$ in $\mathcal{L}(\mathcal{H})$.

Before we turn to the proof we remark that, for $\sigma_{\rm r}(t) = \{e_{\rm r}(t)\}$ and $\{\varphi_\alpha(t)\}_{\alpha=1}^{\ell}$ an orthonormal basis of $\pi_0(t)\mathcal{H}$, the effective Hamiltonian including second order reads

$$h_{\alpha\beta}(t) = e_{\rm r}(t)\delta_{\alpha\beta} \,-\, {\rm i}\,\varepsilon\,\langle\varphi_\alpha(t), \dot\varphi_\beta(t)\rangle \,+\, \frac{\varepsilon^2}{2}\langle\dot\varphi_\alpha(t), R_0(e_{\rm r})\,\dot\varphi_\beta(t)\rangle \,+\, \mathcal{O}(\varepsilon^3)\,,$$

where $R_0(e_{\rm r}) = (H(t) - e_{\rm r}(t))^{-1}\,(1 - \pi_0(t))$. For the unitary $\mathcal{U}^\varepsilon(t)$ one finds

$$\mathcal{U}^{\varepsilon\,*}(t)\pi_{\rm r} = \sum_{\alpha=1}^{\ell}\Big(|\varphi_\alpha(t)\rangle + {\rm i}\varepsilon\, R_0(e_{\rm r})(t)\;|\dot\varphi_\alpha(t)\rangle\Big)\langle\varphi_\alpha(0)| + \mathcal{O}(\varepsilon^2)\,.$$

Proof. In order to apply the general scheme of Chapter 3 it is convenient to introduce the extended space $\mathcal{K} = L^2(\mathbb{R},\mathcal{H}) = \int_{\mathbb{R}}^{\oplus}{\rm d}t\,\mathcal{H}$ and to define the extended Hamiltonian

$$\widehat K = -{\rm i}\varepsilon\partial_t + H(t)$$

which is self-adjoint on the domain $\mathcal{D}(\widehat K) = H^1(\mathbb{R},\mathcal{H}) \subseteq \mathcal{K}$. By following Howland [Ho], we notice that the unitary group ${\rm e}^{-{\rm i}\widehat K\sigma}$, $\sigma\in\mathbb{R}$, is related to the unitary propagator (4.38) through

$$\Big({\rm e}^{-{\rm i}\widehat K\sigma}\psi\Big)\,(t) = U(t,t-\sigma)\psi(t-\sigma)\,. \tag{4.42}$$

Moreover, the unitary group ${\rm e}^{-{\rm i}\widehat K\sigma}$ can now be studied by means of the techniques developed in the previous sections, since $\widehat K$ is nothing but the Weyl quantization of the operator-valued function $K(t,\eta) = \eta + H(t)$, and K belongs to $S^1_1(\mathcal{L}(\mathcal{H}))$.

By assumption $K\in S^1_1$ satisfies assumption $\mathbf{(Gap)}_\sigma$ with $\sigma = 0$. However, because of the simple dependence of $K(t,\eta)$ on η, the conclusion of Theorem 3.2 and of Theorem 3.12 hold still true in a sense to be made precise.

Indeed, by following the proof of Lemma 3.8 one gets a semiclassical symbol $\pi\in S^0_0(\varepsilon,\mathcal{L}(\mathcal{H}))$, depending on t only, such that $[K,\pi]_\sharp \asymp 0$ in $S^1_0(\varepsilon)$. On the other hand,

$$[K,\pi]_\sharp = [H,\pi]_\sharp + [\eta,\pi]_\sharp = [H,\pi]_\sharp - {\rm i}\,\varepsilon\,(\partial_t\pi)$$

where the last equality follows from the fact that $[\eta,\pi]_\sharp$ is the Weyl symbol of $[-{\rm i}\varepsilon\partial_t,\pi(t)] = -{\rm i}\varepsilon\,(\partial_t\pi)\,(t)$. Since both $[H,\pi]_\sharp$ and $\partial_t\pi$ belong to $S^0_0(\varepsilon)$, one concludes that the asymptotic expansion $[K,\pi]_\sharp \asymp 0$ holds true in $S^0_0(\varepsilon)$, and hence $[\widehat K,\widehat\pi] = \mathcal{O}_0(\varepsilon^\infty)$. Finally one defines

$$\Pi^\varepsilon(t) = \frac{\rm i}{2\pi}\int_{|\zeta-1|=\frac12}{\rm d}\zeta\,(\pi(t)-\zeta)^{-1}$$

and finds $\Pi^\varepsilon(\cdot)\in S^0(\varepsilon,\mathcal{L}(\mathcal{H}))$, $\Pi^\varepsilon(t) - \pi(t) = \mathcal{O}_0(\varepsilon^\infty)$ and $[{\rm e}^{-{\rm i}\widehat K\sigma},\Pi^\varepsilon] = \mathcal{O}_0(\varepsilon^\infty|\sigma|)$ as in Section 3.1. Together with (4.42) this implies

$$\operatorname*{ess\,sup}_{t\in\mathbb{R}} \|U(t,t-\sigma)^*\, \Pi^\varepsilon(t)\, U(t,t-\sigma) - \Pi^\varepsilon(t-\sigma)\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}_0(\varepsilon^\infty|\sigma|)\,.$$

However, since $\Pi^\varepsilon(t)$ and $U(t,t')$ are continuous functions of t, the pointwise statement (4.39) follows.

For $u_0(t)$ one can use again Kato's construction [Ka$_2$] and define $u_0(t)$ as the solution of the initial value problem

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u_0^*(t) = [\dot\pi_0(t), \pi_0(t)]\, u_0^*(t)\,, \quad u_0(0) = \mathbf{1}$$

as was done in Section 1.1 to construct the adiabatic time-evolution $U_{\mathrm{a}}^{\varepsilon=1}$. Clearly $u_0(t)$ belongs to $S^0(\mathcal{L}(\mathcal{H}))$. Notice that the same construction does not work in the multidimensional case, since the evolutions in different directions do not commute. $\mathcal{U}^\varepsilon$ can be obtained as in Section 3.2, where the fact that $\pi(t)$ and $u_0(t)$ both depend on t only and not on η simplifies the construction considerably and yields, in particular, a fibered unitary $\mathcal{U}^\varepsilon(t)$.

As in the general setting let the effective Hamiltonian be defined as a resummation of

$$k(\eta,t,\varepsilon) = \big(u \sharp K \sharp u^*\big)(\eta,t,\varepsilon) =: \eta + h(t,\varepsilon)\,,$$

with the explicit expansion (4.41). According to Theorem 3.20 we then have

$$\mathrm{e}^{-\mathrm{i}\widehat{K}\sigma} - \mathcal{U}^{\varepsilon\,*}\, \mathrm{e}^{-\mathrm{i}\widehat{k}\sigma}\, \mathcal{U}^\varepsilon = \mathcal{O}(\varepsilon^\infty|\sigma|)\,,$$

which implies according to (4.42) that

$$\operatorname*{ess\,sup}_{t\in\mathbb{R}} \|U(t,t-\sigma) - \mathcal{U}^{\varepsilon\,*}(t)\, U_{\mathrm{eff}}(t,t-\sigma)\, \mathcal{U}^\varepsilon(t-\sigma)\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}_0(\varepsilon^\infty|\sigma|)\,.$$

The pointwise statement (4.40) follows again from the continuous dependence on t of all involved expressions. □

Remark 4.16. Using the Howland trick one can now easily also treat the case of a Hamiltonian which is the quantization of a time-dependent operator-valued classical symbol $H(q,p,t)$. This is relevant for the Dirac equation, see Section 4.1, or the Bloch electron, see Chapter 5, where the external potential are time-dependent. In these examples the technical modifications in the proofs are straightforward. But the formulation of the results would become even more complicated and hence we treat only the time-independent cases. However, since the change in the effective Hamiltonian is very simple even in the general case, we note here that for time-dependent Hamiltonians Equations (3.39) and (3.40) become

$$h^{(1)}_{\alpha\beta}(t) = E_*(t)\, \delta_{\alpha\beta} + \varepsilon\, h_1(t)_{\alpha\beta}\,, \tag{4.43}$$

with

$$h_1(t)_{\alpha\beta} = \langle \psi_\alpha(t), H_1(t)\,\psi_\beta(t)\rangle - \tfrac{\mathrm{i}}{2}\,\langle \psi_\alpha(t), \{(H_0(t)+E_*(t)), \psi_\beta(t)\}\rangle \\ - \mathrm{i}\,\langle \psi_\alpha(t),\, \partial_t\,\psi_\beta(t)\rangle\,. \tag{4.44}$$

Thus for time-dependent Hamiltonians the subprincipal symbol of the effective Hamiltonian just picks up the additional term $-\mathrm{i}\,\langle \psi_\alpha(t),\, \partial_t\,\psi_\beta(t)\rangle$. See Remark 4.5 for how it contributes in the case of the Dirac equation and Remark 5.15 for the Bloch electron with time-dependent potentials. ♢

4.4 How good is the adiabatic approximation?

In the previous chapters we developed and applied a perturbative scheme to approximate the full quantum dynamics by an effective adiabatic dynamics on almost invariant subspaces. Here "approximate" and "almost" are in the sense of "asymptotically for small ε". All error estimates are of the form that for every $n \in \mathbb{N}$ there is a constant C_n such that

$$\text{“ error ”} < C_n\,\varepsilon^n\,.$$

Hence, no matter what the constants C_n are and no matter how fast C_n may grow as a function of n, one can make the error arbitrarily small at any order of the expansion by choosing ε small enough. But, in applications to real physical systems, we are given a Hamiltonian which is fixed once the units are chosen. In particular, in many examples it does not depend on a small parameter ε in any obvious way. For example the slowly varying external potentials in the Dirac Hamiltonian

$$H_{\mathrm{D}}^{\varepsilon} = \boldsymbol{\alpha}\cdot\big(-\mathrm{i}\nabla_y + A(\varepsilon y)\big) + \boldsymbol{\beta}\,m + \phi(\varepsilon y)\,, \tag{4.45}$$

do not come as functions of εy, they are just some functions of y once physical units are fixed. How can one decide, if some given potentials are varying sufficiently slowly to justify the adiabatic approximation ? Even if one can identify and quantify a small parameter, as the mass ratio $\varepsilon = \sqrt{m/M}$ in the Born-Oppenheimer approximation, there is typically no freedom to vary this parameter in order to to make the errors small. One ends up again with the question: how small must ε be in order to justify the adiabatic approximation and at which order n should one stop the expansion ? Put differently, in applications one is not primarily interested in the order of the error with respect to some parameter, i.e. in the type of mathematical results we obtained. The quantity of interest is the true numerical value of the error, or, at least, good upper bounds to it.

Of course the questions formulated above arise in every perturbative theory that yields asymptotic expansions with respect to a small parameter. A good answer to them makes it necessary to get good bounds on the constants C_n in the asymptotic expansions. Unfortunately it is usually very hard to get such "good" bounds. The construction of the adiabatic expansion based

on pseudodifferential calculus yields, in principle, also the tools to explicitly obtain upper bounds for the constants C_n. However, the results would be neither concise nor even close to optimal, cf. Corollary 2.3 for the simplest case.

Remark 4.17. Using the pseudodifferential calculus for analytic symbols it is possible to obtain bounds on the growth of C_n as a function of n, which are basically of the form $C_n \leq K^n n!$. Sterling's formula together with the choice $n = [g/\varepsilon]$ then yields

$$\text{“ error ”} < \varepsilon^{\frac{g}{\varepsilon}} K^{\frac{g}{\varepsilon}} \left(\frac{g}{\varepsilon}\right)^{\frac{g}{\varepsilon}} = \left(\frac{1}{gK}\right)^{-\frac{g}{\varepsilon}} \leq \mathrm{e}^{-\frac{g}{\varepsilon}}$$

for $0 < g \leq 1/(K\mathrm{e})$. Hence good control on the growth of C_n allows to prove even exponentially small error estimates, cf. [NeSo, MaSo, HaJo$_2$]. However, the error estimates are still in an asymptotic sense and the control on the numerical value of the constants is even less explicit. Hence this does not solve the problem of determining the validity of the adiabatic approximation in a concrete example. ♢

The goal of the present section is very modest. Apart from reminding the reader of the open questions just formulated, we discuss on a heuristic level some qualitative aspects of asymptotic expansions and, in particular, of the adiabatic approximation, which yield some partial answers.

We start by giving a simple answer to the non-problem “What is the exact value of ε in a particular physical system ?” or, more precisely, “What numerical value is assigned to ε when solving the (ε-dependent) effective equations that adiabatic perturbation theory yields for a particular physical system ?”. Given an ε-independent Hamiltonian, as for example a Dirac Hamiltonian of the form

$$H_{\mathrm{D}} = \boldsymbol{\alpha} \cdot \big(-\mathrm{i}\nabla_y + A(y)\big) + \boldsymbol{\beta}\, m + \phi(y)\,,$$

one can always just formally introduce a functional dependence on ε as in (4.45). Now one goes ahead with the adiabatic expansion with respect to ε to the desired order n, determines the constant C_n and in the end sets $\varepsilon = 1$. The numerical error of the adiabatic approximation is then just given by C_n. This shows again that the real question is not so much to quantify ε in a particular physical setting, but to get a good understanding of the constants C_n. But it also shows that in any particular application there will be an optimal order n at which the expansion should be stopped, namely at the order n with the smallest C_n.

Lets be more specific. To each isolated energy band of the principal symbol of the full Hamiltonian H^ε there corresponds an adiabatically decoupled subspace $\Pi^\varepsilon \mathcal{H}$ such that

$$H^\varepsilon = H^\varepsilon_{\mathrm{diag}} + \mathcal{O}(\varepsilon^\infty) := \Pi^\varepsilon\, H^\varepsilon\, \Pi^\varepsilon + (\mathbf{1} - \Pi^\varepsilon)\, H^\varepsilon\, (\mathbf{1} - \Pi^\varepsilon) + \mathcal{O}(\varepsilon^\infty)\,.$$

It could happen that adiabatic decoupling holds exactly, i.e. that $H^\varepsilon = H^\varepsilon_{\rm diag}$. The Dirac equation with small external potentials which do not close the spectral gap of the free Dirac Hamiltonian is an example. Then the almost invariant subspaces, which are usually determined only modulo $\mathcal{O}(\varepsilon^\infty)$, can be identified with spectral subspaces of the Hamiltonian and hence commute with the latter, see Proposition 4.19 below.

However, in general the adiabatically decoupled subspaces are not spectral and transitions between the subspaces are observed. Hence the question for the actual magnitude of such transitions arises. They are governed by the off-diagonal elements of the Hamiltonian,

$$H^\varepsilon_{\rm od} := (\mathbf{1} - \Pi^\varepsilon)\, H^\varepsilon\, \Pi^\varepsilon + \Pi^\varepsilon\, H^\varepsilon\, (\mathbf{1} - \Pi^\varepsilon) = \mathcal{O}(\varepsilon^\infty)\,,$$

which are asymptotically smaller than any power of ε, or, in the case of analytic symbols, even $\mathcal{O}(\mathrm{e}^{-c/\varepsilon})$. While this is conceptually important, it doesn't answer our question on the small but finite magnitude of the transitions which actually occur.

We now sketch a strategy which, once successfully concluded, could yield an answer to this question. Recall that Π^ε was defined in Chapter 3 basically as the quantization of a symbol which is obtained through resummation of the formal symbol $\sum_{n=0}^\infty \varepsilon^n \pi_n(q,p)$. Hence for any fixed ε the projector Π^ε is basically given as the quantization of a finite sum of symbols,

$$\Pi^\varepsilon = \Pi^{(N(\varepsilon))} \approx \sum_{n=0}^{N(\varepsilon)} \varepsilon^n \widehat{\pi}_n\,.$$

Following the terminology of Berry [Be$_2$], we call $\Pi^{(N)}$ the projector on the $N^{\rm th}$ super-adiabatic subspace. By construction we have for the symbol of the off-diagonal part of the Hamiltonian in the block-decomposition with respect to the $N^{\rm th}$ super-adiabatic subspace

$$H^{(N)}_{\rm od} = (\mathbf{1} - \Pi^{(N)})\, H^\varepsilon\, \Pi^{(N)} + \Pi^{(N)}\, H^\varepsilon\, (\mathbf{1} - \Pi^{(N)})$$

that

$$|\, H^{(N)}_{\rm od}(q,p)\,| \le \varepsilon^{N+1}\, C_{N+1}(q,p)\,.$$

For any fixed ε there is then a value for N for which $\varepsilon^{N+1}\, C_{N+1}(q,p)$ is minimal. This value $N_{\rm opt}(\varepsilon)$ for N defines, locally in phase space, the optimal super-adiabatic subspace $\Pi^{(N_{\rm opt}(\varepsilon))}\mathcal{H}$ with respect to which the non-adiabatic transitions are minimal and generated by $H^{(N_{\rm opt}(\varepsilon))}_{\rm od}$. The transitions in the optimal super-adiabatic basis presumably describe the "true" non-adiabatic transitions in the system.

Unfortunately it seems to be very hard to get good control on $H^{(N)}_{\rm od}$ or even on sensible upper bounds for its norm in general. For the time-adiabatic case we refer to the work of Berry and Lim [BeLi$_1$, BeLi$_2$], where the non-adiabatic transitions with respect to the optimal super-adiabatic

basis were analyzed and found to show a universal behavior. In particular the local-in-time transitions within the optimal super-adiabatic basis add up to the correct Landau-Zener formulas when integrated over all times. It is conceivable that also in the general space-adiabatic problem $H_{\rm od}^{(N_{\rm opt}(\varepsilon))}$ has a simple asymptotic form as $\varepsilon \to 0$, which should yield precise information on the true transitions. However, this remains a challenging task for the future.

Remark 4.18. It could happen that the sequence $\varepsilon^{N+1} C_{N+1}$ approaches zero for $N \to \infty$ and hence, that there is no optimal N. However, then the formal series $\sum_{n=0}^{\infty} \varepsilon^n \pi_n(q,p)$ must be indeed convergent and its quantization commutes exactly with H^ε. ♢

We end this section with an extended remark. Clearly one expects that in some cases the almost invariant subspaces are exactly invariant. There seem to be basically two possibilities for this to happen. Either the almost invariant subspace is a spectral subspace of the Hamiltonian or the Hamiltonian is fibered, i.e. its symbol is a function either of p or of q only. In the latter case it can happen because of symmetries that invariant subspaces which are not spectral exist. As an example consider the Bloch electron of Chapter 5 without non-periodic potentials.

A sufficient condition for $\Pi^\varepsilon \mathcal{H}$ to be a spectral subspace of H^ε is the existence of $\lambda_\pm \in \mathbb{R} \cup \{\pm\infty\}$, such that

(i) $\lambda_\pm \notin \sigma(H_0(z))$ for all $z \in \mathbb{R}^{2d}$
(ii) $[\lambda_-, \lambda_+] \cap \sigma_{\rm r}(z) = \sigma_{\rm r}(z)$
(iii) $[\lambda_-, \lambda_+] \cap \big(\sigma\big(H_0(z)\big) \setminus \sigma_{\rm r}(z)\big) = \emptyset$,

where we use the notation of Chapter 3. In this case the spectrum of H^ε is expected to have gaps around λ_+ and λ_- for ε small enough, see Figure 4.1. Then the projection of the almost invariant subspace associated with $\sigma_{\rm r}$ should agree with the spectral projection $\mathbf{1}_{[\lambda_-,\lambda_+]}(H^\varepsilon)$.

While we expect this to be a theorem in the general case, we illustrate the argument in a simple example.

Proposition 4.19. *Assume* **(CG)** *and that the spectrum of $H_0(z)$ consists of two non-degenerate eigenvalues $\sigma(H_0(z)) = E_-(z) \cup E_+(z)$ such that*

$$e_- := \sup_z E_-(z) < \lambda < e_+ := \inf_z E_+(z)$$

for some $\lambda \in \mathbb{R}$. Then, for ε small enough, one has that $\lambda \notin \sigma(\widehat{H})$ and that the projectors $\Pi_\pm^\varepsilon$ on the almost invariant subspaces constructed in the space-adiabatic theorem, Theorem 3.2, agree with the spectral projections of $\widehat{H}$:

$$\Pi_-^\varepsilon = \mathbf{1}_{(-\infty,\lambda)}(\widehat{H}) \quad \text{and} \quad \Pi_+^\varepsilon = \mathbf{1}_{(\lambda,\infty)}(\widehat{H})\,.$$

In particular we have that the almost invariant subspaces $\Pi_\pm^\varepsilon \mathcal{H}$ are exactly invariant.

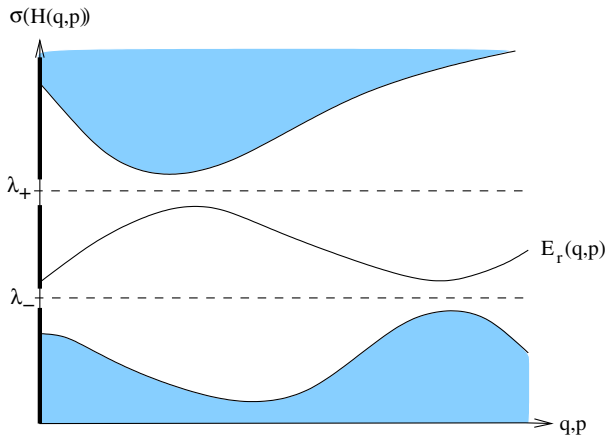

Fig. 4.1. The spectrum of H^ε, indicated by the thick lines on the vertical axis, has gaps around λ_+ and λ_- for sufficiently small ε. Then the almost invariant subspace associated with the spectral band $E_{\rm r}(q,p)$ agrees with the spectral subspace $\mathrm{Ran}\mathbf{1}_{[\lambda_-,\lambda_+]}(H^\varepsilon)$.

Remark 4.20. Recall that the projector Π^ε of Theorem 3.2 is unique only up to a term of order $\mathcal{O}_0(\varepsilon^\infty)$. Hence the equality in Proposition 4.19 must be understood in the sense that it holds for one realization of $\Pi^\varepsilon_\pm$. ♢

Proof. We first show that λ is not in the spectrum of $\widehat{H}$ if ε is sufficiently small. Let U^ε be the unitary operator constructed in Section 3.2, then

$$U^\varepsilon\,\widehat{H}\,U^{\varepsilon\,*} = \begin{pmatrix} \widehat{E}_+ & 0 \\ 0 & \widehat{E}_- \end{pmatrix} + R^\varepsilon =: \widehat{H}_{\rm d} + R^\varepsilon\,,$$

where $\|R^\varepsilon\|_{\mathcal{L}(\mathcal{H})} = \mathcal{O}(\varepsilon)$. According to the semiclassical sharp Garding inequality (cf. Theorem 7.12 in [DiSj]) there is a constant $0 < C < \infty$ such that for ε small enough and all $\psi \in L^2(\mathbb{R}^d)$

$$\langle\psi,\,(\pm\widehat{E}_\pm \mp e_\pm)\,\psi\rangle_{L^2(\mathbb{R}^d)} \geq -\varepsilon C\|\psi\|^2\,.$$

Hence $\sigma(\widehat{E}_+) \geq e_+ - \varepsilon\,C$ and $\sigma(\widehat{E}_-) \leq e_- + \varepsilon C$ and thus

$$\sigma(\widehat{H}_{\rm d}) \subset (-\infty, e_- + \varepsilon C] \cup [e_+ - \varepsilon C, \infty)\,.$$

For ε small enough one thus finds, by standard perturbation theory, that $\sigma(\widehat{H}) \subset I_- \cup I_+$ with two compact disjoint intervals $I_\pm$, which contain the range of $E_\pm$ respectively, but not λ.

Let $\chi_\pm \in C_0^\infty(\mathbb{R})$ with $\chi_\pm|_{I_\pm} = 1$ and $\mathrm{supp}\chi_\pm \cap I_\mp = \emptyset$. Then the spectral projections of $\widehat{H}$ corresponding to $I_\pm$ are given through

$$\mathbf{1}_{I_\pm}(\widehat{H}) = \chi_\pm(\widehat{H})\,.$$

The functional calculus for pseudodifferential operators (cf. Theorem 8.6 in [DiSj]) implies that $\chi_\pm(\widehat{H})$ are also semiclassical pseudodifferential operators with principal symbol $\chi_\pm(H_0(z)) = \pi_{0,\pm}(z)$. The uniqueness part of Lemma 3.8 then insures that the full asymptotic expansion of $\chi_\pm(\widehat{H})$ agrees with the one of $\Pi^\varepsilon_\pm$ and hence that $\chi_\pm(\widehat{H}) - \Pi^\varepsilon_\pm = \mathcal{O}_0(\varepsilon^\infty)$. However, since $\Pi^\varepsilon_\pm$ is unique only up to terms of order $\mathcal{O}_0(\varepsilon^\infty)$, we can as well pick $\Pi^\varepsilon_\pm = \chi_\pm(\widehat{H})$. □

4.5 The Born-Oppenheimer approximation near a conical eigenvalue crossing

It is well known and clearly expected from the foregoing discussions that adiabatic decoupling may break down whenever different eigenvalue bands come too close or cross. In this section we study the Born-Oppenheimer approximation near a conical eigenvalue crossing. Conical crossings are, in a sense, the simplest type of crossing where adiabatic decoupling breaks down at leading order in ε. The generic types of crossings that occur in molecular systems were classified by Hagedorn [Ha$_3$], who also studies propagation of coherent states through such crossings. In particular he finds that adiabatic decoupling breaks down near a conical crossing of the type to be described below. Since then the non-adiabatic propagation of solutions of the Schrödinger equation through eigenvalue crossings has become an active field of research, e.g. [HaJo$_1$, FeGe, FeLa, CLP, LaTe]. The goal of this section is, however, very modest. We will not be concerned with actually determining the non-adiabatic transitions between otherwise decoupled bands near such crossings. Instead we show in a model problem how the higher order corrections to the effective Hamiltonian of the adiabatic approximation become relevant near the crossing point.

To this end we recall that the full quantum Hamiltonian in the molecular setting without magnetic field is

$$\widehat{H}_{\mathrm{BO}} = -\frac{\hbar^2\,\varepsilon^2}{2m}\Delta_x + H_{\mathrm{e}}(x)\,,$$

where $H_{\mathrm{e}}(x)$ is the electronic Hamiltonian, m is the electron mass and $\varepsilon^2 = m/M$ with M the nuclear mass. Since it is always good to remind oneself of the underlying physics, we keep track of all physical constants in this section (in contrast to most of the remainder of the book). Then the Weyl symbol of $\widehat{H}_{\mathrm{BO}}$ is

$$H_{\mathrm{BO}}(q,p) = \frac{1}{2m}p^2 + H_{\mathrm{e}}(q)\,,$$

where quantization is now in the sense of $q \mapsto x$ and $p \mapsto -\mathrm{i}\varepsilon\hbar\nabla_x$.

If the electronic Hamiltonian $H_{\rm e}(q)$ has a (locally) isolated simple eigenvalue band $e_{\rm r}(q)$ with eigenfunction $\chi(q)$, i.e. $H_{\rm e}(q)\,\chi(q) = e_{\rm r}(q)\,\chi(q)$, then the symbol of the effective Born-Oppenheimer Hamiltonian (4.35) on the corresponding reference space reads

$$h_{\rm BO}(q,p) = \frac{1}{2m}\big(p - \varepsilon\,\mathcal{A}(q)\big)^2 + e_{\rm r}(q) + \varepsilon^2\,\Phi(q) + \varepsilon^2\,K(q,p) + \mathcal{O}(\varepsilon^3)\,,$$

with

$$\mathcal{A}(q) = {\rm i}\hbar\langle\,\chi(q), \nabla\chi(q)\rangle\,, \tag{4.46}$$

$$\Phi(q) = \frac{\hbar^2}{2m}\langle\nabla\chi(q),\, \pi_0^\perp(q)\cdot\nabla\chi(q)\rangle\,, \tag{4.47}$$

$$K(q,p) = -\frac{\hbar^2}{m^2}\langle\,p\cdot\nabla\chi(q),\, (H_{\rm e}(q) - e_{\rm r}(q))^{-1}\,\pi_0^\perp(q)\,p\cdot\nabla\chi(q)\rangle\,. \tag{4.48}$$

Here $\pi_0^\perp(q) = \mathbf{1} - \pi_0(q) = \mathbf{1} - |\chi(q)\rangle\langle\chi(q)|$. Notice that $\Phi(q)$, which was termed electric gauge potential in [Be$_3$], and $K(q,p)$ are gauge invariant, i.e. they do not depend on the choice for the eigenfunction $\chi(q)$. More precisely, if one chooses for some smooth real-valued function $\theta(q)$

$$\widetilde{\chi}(q) := {\rm e}^{{\rm i}\theta(q)}\chi(q)$$

instead of $\chi(q)$ for the construction of the unitary mapping to the reference space, then the symbol of the corresponding effective Hamiltonian has the form

$$\widetilde{h}_{\rm BO}(q,p) = \frac{1}{2m}\big(p - \varepsilon\,\widetilde{\mathcal{A}}(q)\big)^2 + e_{\rm r}(q) + \varepsilon^2\,\widetilde{\Phi}(q) + \varepsilon^2\,\widetilde{K}(q,p) + \mathcal{O}(\varepsilon^3)\,,$$

where

$$\widetilde{\mathcal{A}}(q) = {\rm i}\hbar\langle\,\widetilde{\chi}(q), \nabla\widetilde{\chi}(q)\rangle = \mathcal{A}(q) - \hbar\nabla\theta(q)\,,$$

$$\widetilde{\Phi}(q) = \frac{\hbar^2}{2m}\langle\nabla\widetilde{\chi}(q),\, \pi_0^\perp(q)\cdot\nabla\widetilde{\chi}(q)\rangle = \Phi(q)\,,$$

$$\widetilde{K}(q,p) = -\frac{\hbar^2}{m^2}\langle\,p\cdot\nabla\widetilde{\chi}(q),\, (H_{\rm e}(q) - e_{\rm r}(q))^{-1}\,\pi_0^\perp(q)\,p\cdot\nabla\widetilde{\chi}(q)\rangle = K(q,p)\,.$$

The equalities for Φ and K follow from $\pi_0^\perp(q)\chi(q) = 0$. Hence the change in $\mathcal{A}(q)$ is pure gauge and Φ and K remain unchanged.

Since the adiabatic approximation breaks down near eigenvalue crossings, one expects that all the adiabatic correction terms $\mathcal{A}$, Φ and K are singular near such a crossing. It has been demonstrated by Berry and Lim [BeLi$_2$] that the electric gauge potential Φ, which appears also in the conventional Born-Oppenheimer theory as remarked in Section 4.2, is repulsive near such crossings. Obviously $\Phi(q)$ is always positive. Hence, if it diverges at an eigenvalue crossing, it necessarily leads to a repulsive force near such a crossing.

As a consequence, wave functions tend to avoid the crossing region, which presumably improves the validity of the adiabatic approximation.

In the following we will analyze the behavior of K near a conical crossing. It is already clear from the general expression (4.48) that there is an important qualitative difference between the gauge potentials $\mathcal{A}$ and Φ and the dynamical correction K. While the former depend *only* on the geometry of the complex line bundle $\mathbb{C}\chi(q) \mapsto q$, the latter involves the reduced resolvent $(H_{\mathrm{e}}(q) - e_{\mathrm{r}}(q))^{-1}\pi_0^{\perp}(q)$ and thus directly depends also on the energy gap. Hence K dominates Φ in regions of the nucleonic configuration space where the gap between $e_{\mathrm{r}}(q)$ and neighboring eigenvalues is small, but where the variation of the eigenfunction $\chi(q)$ is also small. As can be seen from the general expression (4.48), K has, in contrast to Φ, no fixed sign. In particular it can lead to an attractive force near eigenvalue crossings.

We now compute the effective Hamiltonian for a standard model problem displaying a conical crossing at $q = 0$ in order to illustrate the general observations made above. Let $q = (q_1, q_2)$ and

$$H_{\mathrm{e}}(q) = C \begin{pmatrix} q_1 & q_2 \\ q_2 & -q_1 \end{pmatrix} = C\,|q| \begin{pmatrix} \cos\varphi & \sin\varphi \\ \sin\varphi & -\cos\varphi \end{pmatrix}$$

acting on vectors in $\mathbb{C}^2$. We freely switch between polar and Cartesian coordinates in the following. The eigenvalues of $H_{\mathrm{e}}(q)$ are $e_{\pm}(q) = \pm C|q|$ and a smooth family of eigenfunctions for $q \neq 0$ is given through

$$\phi_+(q) = \mathrm{e}^{\mathrm{i}\varphi/2} \begin{pmatrix} \cos\frac{\varphi}{2} \\ \sin\frac{\varphi}{2} \end{pmatrix} \qquad \text{and} \qquad \phi_-(q) = \mathrm{e}^{\mathrm{i}\varphi/2} \begin{pmatrix} -\sin\frac{\varphi}{2} \\ \cos\frac{\varphi}{2} \end{pmatrix}.$$

A direct computation yields

$$\begin{aligned} \nabla_q \phi_+(q) &= \frac{1}{2|q|}\Big(\phi_-(q) + \mathrm{i}\phi_+(q)\Big)\mathbf{e}_\varphi\,, \\ \nabla_q \phi_-(q) &= \frac{1}{2|q|}\Big(-\phi_+(q) + \mathrm{i}\phi_-(q)\Big)\mathbf{e}_\varphi\,, \end{aligned}$$

where $\mathbf{e}_\varphi = |q|^{-1}(q_2, -q_1) \in \mathbb{R}^2$ in Cartesian coordinates. It is now a simple matter to calculate all the objects appearing in the effective Hamiltonian. One finds

$$\mathcal{A}_{\pm}(q) = \mathrm{i}\hbar\,\langle \phi_{\pm}(q), \nabla_q \phi_{\pm}(q)\rangle = -\frac{\hbar}{2|q|}\mathbf{e}_\varphi\,,$$

$$\Phi_{\pm}(q) = \frac{\hbar^2}{2m}\langle \nabla_q \phi_{\pm}(q), \cdot\pi_{\pm}^{\perp}(q)\,\nabla_q \phi_{\pm}(q)\rangle = \frac{\hbar^2}{8m|q|^2} = \frac{1}{2m}|\mathcal{A}_{\pm}(q)|^2$$

and with

$$(H_{\mathrm{e}}(q) - e_{\pm}(q))^{-1}\pi_{\pm}^{\perp}(q) = \mp\frac{1}{2C|q|}\pi_{\pm}^{\perp}(q)$$

that

$$K_\pm(q,p) = \pm\frac{\hbar^2}{2m^2C|q|}\langle p\cdot\nabla_q\phi_\pm(q),\, \pi_\pm^\perp(q)p\cdot\nabla_q\phi_\pm(q)\rangle = \pm\frac{\hbar^2 L(q,p)^2}{4m^2C|q|^5}\,,$$

where $L(q,p) = q\wedge p = q_1p_2 - q_2p_1$ is the angular momentum.

In summary the symbols of the effective Hamiltonians on the positive resp. negative eigenvalue band are

$$h_\pm(q,p) = \frac{1}{2m}\left(p + \frac{\varepsilon\hbar}{2|q|}\mathbf{e}_\varphi\right)^2 \pm C|q| + \varepsilon^2\frac{\hbar^2}{8m|q|^2} \pm \varepsilon^2\frac{\hbar^2\,L^2(q,p)}{4m^2C|q|^5} + \mathcal{O}(\varepsilon^3)\,.$$

Here the inverse-square potential is the Berry-Lim term, which gives rise to a repulsive inverse-cube force on both bands. The sign of the last term depends on the electronic state. In the positive band it leads to a repulsive force, which is effectively of order $|q|^{-4}$ for fixed momentum and nonzero angular momentum. On the negative band the force is of the same order, but attractive. In both cases it may dominate the contribution from the Berry-Lim term because of the stronger singularity. We remark that the behavior of the sign of K is independent of the specific example, as one can see immediately from (4.48). If two eigenvalue bands $e_n(X) < e_{n+1}(X)$ come very close, the dominant contribution to K_n respectively K_{n+1} comes from the other band. It is positive for K_{n+1} since

$$\begin{aligned}-(H_{\mathrm{e}}(q) - e_{n+1}(q))^{-1}\pi_{n+1}^\perp(q) &= -\sum_{m\neq n+1}(e_m(q) - e_{n+1}(q))^{-1}\pi_m(q)\\ &\approx -(e_n(q) - e_{n+1}(q))^{-1}\pi_n(X) > 0\,,\end{aligned}$$

where $\pi_n(X)$ is the projection onto the eigenspace of $e_n(q)$, and negative for K_n by the analogous argument.

The detailed study of the dynamics of wave packets near conical intersections has attracted considerable interest in the chemical physics literature, see e.g. [FLV] and references therein. The nuclei are often treated semiclassically based on the leading order effective Hamiltonian $\widehat{h}_0 = -\frac{\varepsilon^2\hbar^2}{2m}\Delta_x + e_{\mathrm{r}}(x)$. Although the adiabatic corrections Φ and K are of order $\hbar^2$ with respect to a semiclassical limit, they still might have a considerable impact on classical trajectories which come close to a conical crossing, since they diverge as functions of q. Clearly close to the crossing non-negligible transitions between the two bands occur, an effect which a priori could dominate the influence of the adiabatic corrections Φ and K within the bands. For a classical trajectory $(q(t),p(t))$ passing the crossing at a minimal distance $|q_0|$ with momentum $|p_0|$ the micro-local Landau-Zener formula [CLP] yields a transition ratio

$$T(|q_0|,|p_0|) = \exp\left(-\frac{\pi\, m\, C\,|q_0|^2}{\hbar\,\varepsilon\,|p_0|}\right)\,. \tag{4.49}$$

On the other hand, the relative change in momentum due to $\varepsilon^2\,K$ for such a trajectory is of the order of

$$\frac{\Delta p_0}{|p_0|} \approx \frac{\varepsilon^2 \nabla_q K(|q_0|, |p_0|)\, \Delta t}{|p_0|} \approx \frac{\varepsilon^2 \hbar^2}{m\, C\, |q_0|^3}\,, \tag{4.50}$$

where we chose $\Delta t = |q_0|/v = |q_0| m/|p_0|$. One can now ask if there are trajectories for which transitions are negligible, i.e. $T(|q_0|, |p_0|) \ll 1$, but the influence of K is significant, i.e. $\Delta p_0/p_0 \approx \mathcal{O}(1)$. Solving (4.50) ≈ 1 for $|q_0|$ we find that the influence of K is significant for trajectories passing with $|q_0| \approx (\varepsilon^2 \hbar^2/mC)^{1/3}$. Inserted into (4.49) this yields that $T(|q_0|, |p_0|) \ll 1$ whenever $|p_0| \ll \pi (mC\varepsilon\hbar)^{1/3}$. This heuristic argument shows that for suitable choices of parameters it can certainly happen that the higher order adiabatic correction become relevant in regions of phase space, where the non-adiabatic transitions are still negligible.

While we plan to investigate the influence of Φ and K on the semiclassical dynamics near conical crossings in the future, we conclude with the following observation. Numerical solutions of the time-dependent Schrödinger equation with the above model Hamiltonian found in [LaTe] show an interesting behavior. An initial Gaussian wave packet starting in the positive band moves across the intersection and, as one expects, splits into a component remaining on the positive band and one emerging and propagating on the negative band. However, the wave function emerging on the negative band has a rather pronounced cusp at $q = 0$. We regard this as a manifestation of the singular attractive force coming from K_-.

5 Quantum dynamics in periodic media

A central problem of solid state physics is to understand the motion of electrons in a periodic potential which is generated by the ionic cores. While this problem is quantum mechanical, many electronic properties of solids can be understood already in the semiclassical approximation [AsMe, Ko, Za]. One argues that for suitable wave packets, which are spread over many lattice spacings, the main effect of a periodic potential V_Γ on the electron dynamics corresponds to changing the dispersion relation from the free kinetic energy $E_{\text{free}}(p) = \frac{1}{2}p^2$ to the modified kinetic energy $E_n(p)$ given by the n^{th} Bloch function. Otherwise the electron responds to slowly varying external potentials A, ϕ as in the case of a vanishing periodic potential. Thus the semiclassical equations of motion are

$$\dot{q} = \nabla E_n(\pi)\,, \qquad \dot{\pi} = -\nabla\phi(q) + \dot{q} \times B(q)\,, \tag{5.1}$$

where $\pi = p - A(q)$ is the kinetic momentum and $B = \nabla \times A$ is the magnetic field. (As in the previous chapters we choose units in which the Planck constant $\hbar$, the speed c of light, and the mass m of the electron are equal to one, and absorb the charge e into the potentials.) The corresponding equations of motion for the canonical variables (q, p) are generated by the Hamiltonian

$$H_{\text{sc}}(q,p) = E_n\big(p - A(q)\big) + \phi(q)\,,$$

where q is the position and p the quasi-momentum of the electron. Note that there is a semiclassical evolution for each Bloch band separately.

In this chapter we present results from Panati, Spohn, Teufel [PST$_3$], where adiabatic perturbation theory is applied in order to understand on a mathematical level how these semiclassical equations emerge from the underlying Schrödinger equation

$$\mathrm{i}\,\partial_s\,\psi(x,s) = \Big(\tfrac{1}{2}\big(-\mathrm{i}\nabla_x - A(\varepsilon x)\big)^2 + V_\Gamma(x) + \phi(\varepsilon x)\Big)\,\psi(x,s) \tag{5.2}$$

in the limit $\varepsilon \to 0$ at leading order. In addition the order ε correction to (5.1) is established, see Equation (5.4). As an additional motivation for the detailed study which follows let us quote from the solid states physics text book [AsMe], whose authors consider the derivation of (5.1) from (5.2) a "formidable task".

S. Teufel: LNM 1821, pp. 141–171, 2003.

In (5.2) the potential $V_\Gamma : \mathbb{R}^d \to \mathbb{R}$ is periodic with respect to some regular lattice Γ generated through the basis $\{\gamma_1, \ldots, \gamma_d\}$, $\gamma_j \in \mathbb{R}^d$, i.e.

$$\Gamma = \Big\{ x \in \mathbb{R}^d : x = \textstyle\sum_{j=1}^d \alpha_j \gamma_j \ \text{ for some } \alpha \in \mathbb{Z}^d \Big\}$$

and $V_\Gamma(\cdot + \gamma) = V_\Gamma(\cdot)$ for all $\gamma \in \Gamma$. The lattice spacing defines the microscopic spatial scale. The external potentials $A(\varepsilon x)$ and $\phi(\varepsilon x)$, with $A : \mathbb{R}^d \to \mathbb{R}^d$ and $\phi : \mathbb{R}^d \to \mathbb{R}$, are slowly varying on the scale of the lattice, as expressed through the dimensionless scale parameter ε, $\varepsilon \ll 1$. In particular, this means that the external fields are weak compared to the fields generated by the ionic cores, a condition which is satisfied for real metals even for the strongest external electrostatic fields available and for a wide range of magnetic fields, cf. [AsMe], Chapter 12.

Note that, as in the study of the Dirac equation in Section 4.1, the external forces due to A and ϕ are of order ε and therefore have to act over a time of order ε^{-1} to produce finite changes, which is again taken as the definition of the macroscopic time scale. Hence, we will be interested in solutions of (5.2) for macroscopic times, but we will work mostly in the microscopic coordinates (x, s). For sake of comparison we recall that the macroscopic space-time scale (x', t) is defined through $x' = \varepsilon x$ and $t = \varepsilon s$. With this change of scale Equation (5.2) reads

$$\mathrm{i}\,\varepsilon\,\partial_t\,\psi^\varepsilon(x', t) = \Big(\tfrac{1}{2}\big(-\mathrm{i}\varepsilon\nabla_{x'} - A(x')\big)^2 + V_\Gamma(x'/\varepsilon) + \phi(x') \Big)\,\psi^\varepsilon(x', t) \quad (5.3)$$

with initial conditions $\psi^\varepsilon(x') = \varepsilon^{-d/2}\psi(x'/\varepsilon)$. If $V_\Gamma = 0$, Equation (5.3) is the usual semiclassical limit with ε set equal to $\hbar$.

The problem of deriving (5.1) from the Schrödinger equation (5.2) in the limit $\varepsilon \to 0$ has been attacked along several routes. In the physics literature (5.1) is usually accounted for by constructing suitable semiclassical wave packets. We refer to [Lu, Ko, Za, Wa] and Appendix C. The few mathematical approaches to the time-dependent problem (5.3) extend techniques from semiclassical analysis, as the Gaussian beam construction [GRT, DGR], or Wigner measures [GMMP, MMP], the latter being carried out only for vanishing external potential. The large time asymptotics of the solutions to (5.3) without external potentials is studied in [AsKn] and the scattering theory is developed in [GeNi].

Although neither (5.2) nor (5.3) has the space-adiabatic form (1.1), the underlying physics clearly indicate that the step from (5.2) to (5.1) involves actually two limits. Semiclassical behavior can only emerge if a Bloch band is separated by a gap from the other bands and thus the corresponding subspace decouples adiabatically from its orthogonal complement. Hence we must reformulate (5.2) as a space-adiabatic problem. This has been done first in [HST], where the semiclassical model (5.1) is derived for the case of zero magnetic field using the techniques from Chapter 2.

The present chapter is, in spirit, a continuation of the program started in [HST] to the case of both, external magnetic and electric fields. This is possible by reformulating the problem in such a way that the general scheme developed in Chapter 3 can be applied with some modifications. The results we obtain this way constitute the first derivation of the semiclassical model in this generality. In particular, for non-degenerate bands we are able to compute the first order corrections in the small parameter ε to the semiclassical equations (5.1) based on a semiclassical analysis of the effective Hamiltonian on the reference space. The corrected equations including all terms of first order in ε read

$$\begin{aligned} \dot{q} &= \nabla_\pi \Big(E_n(\pi) - \varepsilon\, B(q) \cdot M_n(\pi) \Big) - \varepsilon\, \dot{\pi} \times \Omega_n(\pi)\,, \\ \dot{\pi} &= -\nabla_q \Big(\phi(q) - \varepsilon\, B(q) \cdot M_n(\pi) \Big) + \dot{q} \times B(q)\,. \end{aligned} \tag{5.4}$$

The Berry connection of the eigenspace-bundle corresponding to the Bloch band E_n enters in a gauge-invariant way through its curvature $\Omega_n = \mathrm{d}\mathcal{A}_n$ and through the effective magnetic moment M_n. The precise definitions of the new terms are given below in Corollary 5.12.

The first equation in (5.4) agrees with the expression found by Sundaram and Niu [SuNi] based on coherent state solutions, while the correction in the second equation in (5.4) is new. This nicely illustrates our point that it is advantageous to work with effective equations of motion as much as possible, as opposed to directly construct approximate solutions. While the higher order corrections in the equations of motion (5.4) allow for an immediate physical interpretation, the higher order corrections obtained for coherent state solutions in [SuNi] or for WKB solutions in [DGR] do not yield (5.4) in any straightforward way.

The dynamical system (5.1) is of interest in its own, c.f. [MaNo] and references therein, due to the nontrivial topology of the underlying phase space, and we hope that the corrections in (5.4) give rise to further investigations. We discuss the equations (5.4) only shortly at the beginning of Section 5.3, where we show in particular, that they are Hamiltonian with respect to a non-standard symplectic form. One concrete physical application of the refined semiclassical equations (5.4) is a quantitative theory for the anomalous Hall effect [JNM].

Remark 5.1. In the presence of a strong external magnetic field with rational flux per unit cell one formally obtains semiclassical equations identical to (5.4), except that the Bloch band E_n must be replaced by one of the magnetic sub-bands. As on striking consequence they provide the semiclassical explanation for the quantization of the Hall conductivity. More precisely, for spatial dimension $d = 2$, $\phi(q) = -\mathcal{E} \cdot q$, $B(q) = 0$, the equations of motion (5.4) become $\dot{q} = \nabla_\pi E_n(\pi) + \mathcal{E}^\perp \Omega_n(\pi)$, $\dot{\pi} = \mathcal{E}$, where Ω_n is now scalar and

$\mathcal{E}^\perp$ is $\mathcal{E}$ rotated by $\pi/2$. We assume initially $\pi(0) = k$ and a completely filled band, which means to integrate with respect to k over the first Brillouin zone. Then the average current for band n is given by

$$j_n = \int \mathrm{d}k\, \dot{q}(k) = \int \mathrm{d}k \left(\nabla_k E_n(k) - \mathcal{E}^\perp \Omega_n(k)\right) = -\mathcal{E}^\perp \int \mathrm{d}k\, \Omega_n(k)\,.$$

$\int \mathrm{d}k\, \Omega_n(k)$ is the Chern number of the magnetic Bloch bundle and as such an integer. Further applications related to the semiclassical first order corrections are the anomalous Hall effect [JNM] and the thermodynamics of the Hofstadter model [GaAv]. ♢

Since the precise statements of our results require considerable technical preparations, they are postponed to Section 5.2. At this point we only give an informal outline of the results, concluding with the theorem connecting (5.2) and (5.4).

Under Assumption (A_1) the Hamiltonian

$$H^\varepsilon = \tfrac{1}{2}\big(-\mathrm{i}\nabla_x - A(\varepsilon x)\big)^2 + V_\Gamma(x) + \phi(\varepsilon x)\,. \tag{5.5}$$

is self-adjoint on the domain $H^2(\mathbb{R}^d)$ and hence generates solutions to (5.2) in $\mathcal{H} := L^2(\mathbb{R}^d)$ through the unitary group $\mathrm{e}^{-\mathrm{i}H^\varepsilon s}$, $s \in \mathbb{R}$. The natural representation for applying space-adiabatic theory along the lines of Chapter 3 is the Bloch-Floquet representation, which is introduced in Section 5.1. In Section 5.2 we then present and prove the main results of the space-adiabatic approximation. The key observation for applying space-adiabatic perturbation theory is that the Hamiltonian H^ε can be written, after a suitable Bloch-Floquet transformation, as the Weyl quantization of an operator valued symbol. However, the underlying Hilbert space is not of the form $L^2(\mathbb{R}^d, \mathcal{H}_\mathrm{f})$, as for usual Weyl quantization, but $L^2(M^*, \mathcal{H}_\mathrm{f})$, where M^* is the first Brillouin zone, the fundamental domain of the dual lattice Γ^*. And the symbols are not functions on the phase space $\mathbb{R}^d \times \mathbb{R}^d$, but on $M^* \times \mathbb{R}^d$. Hence a suitable version of the parameter dependent pseudodifferential calculus needs to be developed in Appendix B.

Before entering the technical details let us state the theorem relating the Schrödinger equation (5.2) and the corrected semiclassical model (5.4). To this end we need a few extra notations. By Γ^* we denote the dual lattice of Γ and $\Phi_n^t : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is the flow corresponding to (5.4). For a comparison with the quantum dynamics we need to switch back to canonical coordinates in (5.4). After the change of coordinates $(q, \pi) \mapsto (q, p) = (q, \pi + A(q))$ the flow in canonical coordinates is described by

$$\overline{\Phi}_n^t(q,p) = \Big(\Phi_{n\,q}^t\big(q, p - A(q)\big),\, \Phi_{n\,\pi}^t\big(q, p - A(q)\big) + A(q)\Big)\,.$$

Our theorem says that the semiclassical observables are given through pseudodifferential operators with Γ^*-periodic symbols and that the Heisenberg

time-evolution of such an observable, projected onto the corresponding adiabatic subspace $\Pi_n^\varepsilon \mathcal{H}$, is approximated by transporting the symbol along the flow (5.4) up to an error of order ε^2.

Theorem 5.2. *Let E_n be an isolated, non-degenerate Bloch band, see Definition 5.7, and let the potentials satisfy Assumption (A_1). Let $a \in C_{\mathrm{b}}^\infty(\mathbb{R}^{2d})$ be Γ^*-periodic in the second argument, i.e. $a(q, p + \gamma^*) = a(q, p)$ for all $\gamma^* \in \Gamma^*$, and $\widehat{a} = a(\varepsilon x, -\mathrm{i}\nabla_x)$ be its Weyl quantization. Then for each finite time-interval $I \subset \mathbb{R}$ there is a constant $C < \infty$ such that for $t \in I$*

$$\left\| \Pi_n^\varepsilon \left(\mathrm{e}^{\mathrm{i}H^\varepsilon t/\varepsilon}\, \widehat{a}\, \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} - \widehat{a \circ \overline{\Phi}_n^t} \right) \Pi_n^\varepsilon \right\|_{\mathcal{L}(L^2(\mathbb{R}^d))} \leq \varepsilon^2\, C\,.$$

In particular, for $\psi_0 \in \Pi_n^\varepsilon \mathcal{H}$ we have that

$$\left| \left\langle \psi_0,\, \mathrm{e}^{\mathrm{i}H^\varepsilon t/\varepsilon}\, \widehat{a}\, \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}\, \psi_0 \right\rangle - \left\langle \psi_0,\, \widehat{a \circ \overline{\Phi}_n^t}\, \psi_0 \right\rangle \right| \leq \varepsilon^2\, C\, \|\psi_0\|^2\,.$$

To our knowledge, Theorem 5.2 is the first rigorous result relating the full time-dependent Schrödinger equation (5.2) to the semiclassical model (5.1) for general external magnetic and electric fields and the first result to include the first order corrections (5.4). For an elementary discussion on how this results relates to other approaches to the semiclassical problem (5.3) see [Te$_3$].

Remark 5.3. Note that the statement of Theorem 5.2 differs from the Egorov theorem formulated in Corollary 3.29 in two ways. In order to obtain the improved error estimate in Theorem 5.2, $\mathcal{O}(\varepsilon^2)$ instead of $\mathcal{O}(\varepsilon)$, we introduced an ε-dependent classical flow (recall that (5.4) depends on ε). However, since the classical observables in the original representation commute with Π_n^ε only at leading order, we need to project them onto the almost invariant subspace from both sides, cf. the discussion at the end of Section 3.4.3. ♢

Remark 5.4. The spectral problem for H^ε was solved in [GMS], with predecessors [BeRa, Bu, HeSj, Nen$_3$]. In this case the goal is to obtain an effective Hamiltonian with the same spectrum as H^ε closed to some prescribed energy, see also Appendix C. ♢

The derivation of the semiclassical equations of motion (5.1) from the effective quantum Hamiltonian of Section 5.2 and the proof of Theorem 5.2 is given in Section 5.3.

5.1 The periodic Hamiltonian

In order to formulate our assumptions and our results we first need to recall several well known facts about the periodic Hamiltonian

$$H_{\rm per} := -\frac{1}{2}\Delta + V_\Gamma\,,$$

i.e. about (5.5) without the non-periodic perturbations A and ϕ.

The potential V_Γ is periodic with respect to the lattice Γ. Its dual lattice Γ^* is defined as the lattice generated by the dual basis $\{\gamma_1^*, \ldots, \gamma_d^*\}$ determined through the conditions $\gamma_i \cdot \gamma_j^* = 2\pi\delta_{ij}$, $i, j \in \{1, \ldots, d\}$. The centered fundamental domain of Γ is denoted by

$$M = \left\{ x \in \mathbb{R}^d : x = \textstyle\sum_{j=1}^d \alpha_j\, \gamma_j \ \text{ for } \alpha_j \in [-\frac{1}{2}, \frac{1}{2}] \right\},$$

and analogously the centered fundamental domain of Γ^* is denoted by M^*. In solid state physics the set M^* is called the *first Brillouin zone*. In the following M^* is always equipped with the *normalized* Lebesgue measure denoted by $\mathrm{d}k$. We introduce the notation $x = [x] + \gamma$ for the a.e. unique decomposition of $x \in \mathbb{R}^d$ as a sum of $[x] \in M$ and $\gamma \in \Gamma$. We use the same brackets for the analogous splitting $k = [k] + \gamma^*$.

The Bloch-Floquet transform of a function $\psi \in \mathcal{S}(\mathbb{R}^d)$ is defined as

$$(\mathcal{U}\psi)(k, y) := \sum_{\gamma \in \Gamma} \mathrm{e}^{-\mathrm{i}(y+\gamma)\cdot k} \psi(y + \gamma), \ \ (k, y) \in \mathbb{R}^{2d} \tag{5.6}$$

and one directly reads off from (5.6) the following periodicity properties:

$$\big(\mathcal{U}\psi\big)(k, y + \gamma) = \big(\mathcal{U}\psi\big)(k, y) \quad \text{ for all } \quad \gamma \in \Gamma\,, \tag{5.7}$$

$$\big(\mathcal{U}\psi\big)(k + \gamma^*, y) = \mathrm{e}^{-\mathrm{i}y\cdot\gamma^*} \big(\mathcal{U}\psi\big)(k, y) \quad \text{ for all } \quad \gamma^* \in \Gamma^*\,. \tag{5.8}$$

Remark 5.5. In the present context the Bloch-Floquet transformation is also called Zak transformation, or Lifshitz-Gelfand-Zak transformation. Since priorities are not obvious here, we stick to the "Bloch-Floquet"-terminology. ♢

From (5.7) it follows that, for any fixed $k \in \mathbb{R}^d$, $\big(\mathcal{U}\psi\big)(k, \cdot)$, is a Γ-periodic function and can then be regarded as an element of $L^2(\mathbb{T}^d)$, $\mathbb{T}^d$ being the flat torus $\mathbb{R}^d/\Gamma$. For general results on Floquet theory we refer e.g. to [Ku].

Equation (5.8) involves a unitary representation of the group of lattice translation on Γ^* (denoted again as Γ^* with a little abuse of notation), given by

$$\tau : \Gamma^* \to \mathcal{U}(L^2(\mathbb{T}^d))\,, \quad \gamma^* \mapsto \tau(\gamma^*)\,,$$

where $\tau(\gamma^*)$ is given by multiplication with $\mathrm{e}^{\mathrm{i}\, y\cdot\gamma^*}$ in $L^2(\mathbb{T}^d, \mathrm{d}y)$. It will prove convenient to introduce the Hilbert space

$$\mathcal{H}_\tau := \left\{ \psi \in L^2_{\rm loc}(\mathbb{R}^d, L^2(\mathbb{T}^d)) : \ \psi(k - \gamma^*) = \tau(\gamma^*)\, \psi(k) \right\}, \tag{5.9}$$

equipped with the inner product

$$\langle \psi,\, \varphi \rangle_{\mathcal{H}_\tau} = \int_{M^*} \mathrm{d}k\, \langle \psi(k),\, \varphi(k) \rangle_{L^2(\mathbb{T})}\,.$$

Notice that if one considers the trivial representation, i.e. $\tau \equiv \mathbf{1}$, then $\mathcal{H}_\tau$ is nothing but a space of Γ^*-periodic vector-valued functions over $\mathbb{R}^d$.

Obviously, there is a natural isomorphism to $L^2(M^*, L^2(\mathbb{T}^d))$ from $\mathcal{H}_\tau$ given by restriction from $\mathbb{R}^d$ to M^*, and with inverse given by τ-equivariant continuation, as suggested by (5.8). The reason for working with $\mathcal{H}_\tau$ instead of $L^2(M^*, L^2(\mathbb{T}^d))$ is twofold. First of all it allows to apply the pseudodifferential calculus as developed in Appendix B. On the other hand it makes statements about domains of operators more transparent as we shall see.

The map defined by (5.6) extends to a unitary operator

$$\mathcal{U} : L^2(\mathbb{R}^d) \to \mathcal{H}_\tau \cong L^2(M^*, L^2(\mathbb{T}^d)) \cong L^2(M^*) \otimes L^2(\mathbb{T}^d)\,.$$

The facts that $\mathcal{U}$ is an isometry and that $\mathcal{U}^{-1}$ given through

$$\big(\mathcal{U}^{-1}\varphi\big)(x) = \int_{M^*} \mathrm{d}k\; \mathrm{e}^{\mathrm{i}x\cdot k}\, \varphi(k, [x]) \tag{5.10}$$

satisfies $\mathcal{U}^{-1}\mathcal{U}\psi = \psi$ for $\psi \in \mathcal{S}(\mathbb{R}^d)$ can be checked by direct calculation. It is also straightforward to check that $\mathcal{U}^{-1}$ extends to an isometry from $\mathcal{H}_\tau$ to $L^2(\mathbb{R}^d)$. Hence $\mathcal{U}^{-1}$ must be injective and as a consequence U must be surjective and thus unitary.

In order to determine the Bloch-Floquet transform of operators like the full Hamiltonian (5.5), we need to discuss how differential and multiplication operators behave under Bloch-Floquet transformation. The following assertions follow in a straightforward way from the definition (5.6). Let $P = -\mathrm{i}\nabla_x$ with domain $H^1(\mathbb{R}^d)$ and Q be multiplication with x on the maximal domain, then

$$\mathcal{U}\, P\, \mathcal{U}^{-1} = \mathbf{1} \otimes -\mathrm{i}\nabla_y^{per} + k \otimes \mathbf{1} \tag{5.11}$$

$$\mathcal{U}\, Q\, \mathcal{U}^{-1} = \mathrm{i}\nabla_k^{\tau}\,, \tag{5.12}$$

where $-\mathrm{i}\nabla_y^{per}$ is equipped with periodic boundary conditions or, equivalently, operating on the domain $H^1(\mathbb{T}^d)$. The domain of $\mathrm{i}\nabla_k^{\tau}$ is $\mathcal{H}_\tau \cap H^1_{\mathrm{loc}}(\mathbb{R}^d, L^2(\mathbb{T}))$, i.e. it consists of distributions in $H^1(M^*, L^2(\mathbb{T}^d))$ which satisfy the y-dependent boundary condition associated with (5.8).

The central feature of the Bloch-Floquet transformation is, however, that multiplication with a Γ periodic function like V_Γ is mapped into multiplication with the same function, i.e. $\mathcal{U}\, V_\Gamma(x)\, \mathcal{U}^{-1} = \mathbf{1} \otimes V_\Gamma(y)$.

For later use we remark that the following relations can be checked using the definitions (5.6) and (5.10):

$$\begin{aligned} \psi \in H^m(\mathbb{R}^d)\,,\ m \geq 0 \quad &\Longleftrightarrow \quad \mathcal{U}\psi \in L^2(M^*, H^m(\mathbb{T})) \\ \langle x \rangle^m \psi(x) \in L^2(\mathbb{R}^d)\,,\ m \geq 0 \quad &\Longleftrightarrow \quad \mathcal{U}\psi \in \mathcal{H}_\tau \cap H^m_{\mathrm{loc}}(\mathbb{R}^d, L^2(\mathbb{T}))\,. \end{aligned}$$

Remark 5.6. Often the Bloch-Floquet transformation is defined for $\psi \in \mathcal{S}(\mathbb{R}^d)$ as

$$(\widetilde{\mathcal{U}}\psi)(k,y) := \sum_{\gamma\in\Gamma} \mathrm{e}^{-\mathrm{i}y\cdot k}\psi(y+\gamma), \quad (k,y)\in\mathbb{R}^{2d}\,. \tag{5.13}$$

In contrast to (5.6), functions in the range of $\widetilde{\mathcal{U}}$ are periodic in k and quasi-periodic in y:

$$\big(\widetilde{\mathcal{U}}\psi\big)(k,y+\gamma) = \mathrm{e}^{\mathrm{i}k\cdot\gamma}\,\big(\widetilde{\mathcal{U}}\psi\big)(k,y) \quad \text{for all} \quad \gamma\in\Gamma \tag{5.14}$$

$$\big(\widetilde{\mathcal{U}}\psi\big)(k+\gamma^*,y) = \big(\widetilde{\mathcal{U}}\psi\big)(k,y) \quad \text{for all} \quad \gamma^*\in\Gamma^*\,. \tag{5.15}$$

Our choice of $\mathcal{U}$ instead of $\widetilde{\mathcal{U}}$ comes from the fact, that the transform of the gradient has a domain which is independent of $k\in M^*$, cf. (5.11). This is, as we shall see, essential for an application of the pseudodifferential calculus of Appendix B. ♢

For the Bloch-Floquet transform of the free Hamiltonian one finds

$$\mathcal{U}\,H_{\mathrm{per}}\,\mathcal{U}^{-1} = \int_{M^*}^{\oplus} \mathrm{d}k\, H_{\mathrm{per}}(k)$$

with

$$H_{\mathrm{per}}(k) = \frac{1}{2}\big(-\mathrm{i}\nabla_y + k\big)^2 + V_\Gamma(y)\,, \quad k\in M^*\,. \tag{5.16}$$

For fixed $k\in M^*$ the operator $H_{\mathrm{per}}(k)$ acts on $L^2(\mathbb{T}^d)$ with domain $H^2(\mathbb{T}^d)$ independent of $k\in M^*$, whenever the following assumption on the potential is satisfied.

Assumption ($\mathbf{A}_1$). *We assume that V_Γ is infinitesimally bounded with respect to $-\Delta$ and that $\phi\in C^\infty_{\mathrm{b}}(\mathbb{R}^d,\mathbb{R})$ and $A_j\in C^\infty_{\mathrm{b}}(\mathbb{R}^d,\mathbb{R})$ for any $j\in\{1,\dots,d\}$.*

From this assumption it follows in particular that H^ε is self-adjoint on $H^2(\mathbb{R}^d)$. The previous assumption excludes the case of globally constant electric and magnetic field. However, since we are not concerned with the spectral analysis of H^ε, but with the dynamics of states for large but finite times, locally constant fields serve us as well.

The band structure of the fibered spectrum of H_{per} is crucial for the following and a more detailed discussion can be found in [Wi]. The resolvent $R^0_\lambda = (H_0(k)-\lambda)^{-1}$ of the operator $H_0(k) = \frac{1}{2}\big(-\mathrm{i}\nabla_y + k\big)^2$ is compact for fixed $k\in M^*$. Since, by assumption, $R_\lambda V_\Gamma$ is bounded, also $R_\lambda = (H_{\mathrm{per}}(k)-\lambda)^{-1} = R^0_\lambda + R_\lambda V_\Gamma R^0_\lambda$ is compact. As a consequence $H_{\mathrm{per}}(k)$ has purely discrete spectrum with eigenvalues of finite multiplicity which accumulate at infinity. For definiteness the eigenvalues are enumerated according to their magnitude, $E_1(k)\le E_2(k)\le E_3(k)\le\dots$ and repeated according to their multiplicity. The corresponding normalized eigenfunctions

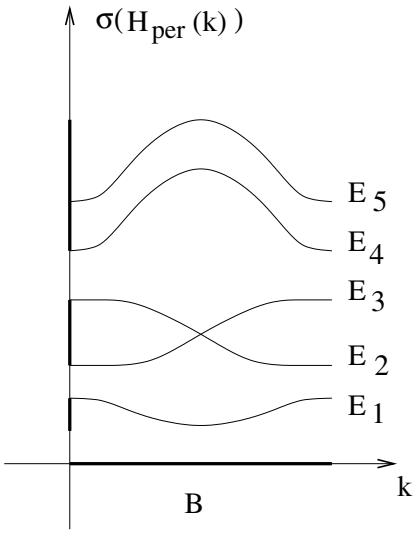

Fig. 5.1. Schematic view of the Bloch bands: E_1, E_4 and E_5 are isolated bands, while $\{E_2, E_3\}$ is an isolated family of bands.

$\{\varphi_n(k)\}_{n\in\mathbb{N}} \subset H^2(\mathbb{T}^d)$ are called Bloch functions and form, for any fixed k, an orthonormal basis of $L^2(\mathbb{T}^d)$. We will call $E_n(k)$ the n^{th} band function or just the n^{th} band. Notice that, with this choice of the labelling, $E_n(k)$ and $\varphi_n(k)$ are generally *not* smooth functions of k if eigenvalue crossings are present. Since

$$H_{\text{per}}(k-\gamma^*) = \tau(\gamma^*)\, H_{\text{per}}(k)\, \tau(\gamma^*)^{-1}\,, \tag{5.17}$$

the band functions $E_n(k)$ are periodic with respect to Γ^*, cf. Figure 5.1.

Definition 5.7. *We say that a band $E_n(k)$ or a family of bands $\{E_n(k)\}_{n\in\mathcal{I}}$, $\mathcal{I} = [I_-, I_+] \cap \mathbb{N}$, is **isolated** resp. satisfies the* **gap condition**, *if*

$$\inf_{k\in M^*} \operatorname{dist}\Big(\bigcup_{n\in\mathcal{I}} \{E_n(k)\},\ \bigcup_{m\notin\mathcal{I}} \{E_m(k)\} \Big) =: C_{\text{g}} > 0\,.$$

Remark 5.8. A warning concerning the terminology is in order. It is often not the function $E_n(k)$ which is called the Bloch band, but its projection onto the energy axis, cf. Figure 5.1, i.e. the set

$$\overline{E}_n := \overline{\bigcup_{k\in M^*} E_n(k)} \subset \sigma(H_{\text{per}})\,.$$

Within such a context a band is called isolated whenever $\overline{E}_n \cap \overline{E}_{n\pm1} = \emptyset$, i.e. if $\overline{E}_n$ is separated by gaps from the remainder of the spectrum of H_{per}. Clearly this notion of "isolated bands" is much more restrictive than the one of Definition 5.7. ♢

For the following we fix an index set $\mathcal{I} \subset \mathbb{N}$ corresponding to an isolated family of bands. Let $P_{\mathcal{I}}(k)$ be the spectral projector of $H_{\mathrm{per}}(k)$ corresponding to the eigenvalues $\{E_n(k)\}_{n\in\mathcal{I}}$, then $P_{\mathcal{I}} := \int_{M^*}^{\oplus} \mathrm{d}k\, P_{\mathcal{I}}(k)$ is the projector on the given isolated Bloch band.

In terms of Bloch functions, one has that $P_{\mathcal{I}}(k) = \sum_{n\in\mathcal{I}} |\varphi_n(k)\rangle\langle\varphi_n(k)|$. However, in general, $\varphi_n(k)$ are not smooth functions of k at eigenvalue crossings, while $P_{\mathcal{I}}(k)$ is a smooth function of k because of the gap condition. Moreover, from (5.17) it follows that

$$P_{\mathcal{I}}(k-\gamma^*) = \tau(\gamma^*)\, P_{\mathcal{I}}(k)\, \tau(\gamma^*)^{-1}\,.$$

In the unphysical case of $d > 3$ we will need an additional assumption in order to construct the mapping to the reference space.

Assumption (A_2). *If $d > 3$ and if the isolated family of Bloch bands $\{E_n(k)\}_{n\in\mathcal{I}}$ is degenerate in the sense that $\ell := |\mathcal{I}| > 1$, then we assume that there exists an orthonormal basis $\{\psi_j(k)\}_{j=1}^{\ell}$ of $\mathrm{Ran}P_{\mathcal{I}}(k)$ whose elements are smooth and τ-equivariant with respect to k, i.e. $\psi_j(k-\gamma^*) = \tau(\gamma^*)\psi_j(k)$ for all $j \in \{1,\dots,\ell\}$ and $\gamma^* \in \Gamma^*$.*

As to be discussed in Section 5.3.2, this assumption is a proper reformulation of the assumption on the existence of the unitary u_0 in Section 3.2.

In the special but important case in which the family of bands consist of a single isolated ℓ-fold degenerate eigenvalue (i.e. $E_n(k) = E_*(k)$ for every $n \in \mathcal{I}$, $|\mathcal{I}| = \ell$), Assumption (A_2) is equivalent to the existence of an orthonormal basis consisting of smooth and τ-equivariant Bloch functions. In the general case, in which *eigenvalue crossings* within the isolated family of bands are present, Assumption (A_2) is weaker, since it is not required that $\psi_j(k)$ is an eigenfunction of the free Hamiltonian $H_{\mathrm{per}}(k)$, but only of the corresponding eigenprojection $P_{\mathcal{I}}(k)$.

Remark 5.9. From the geometrical viewpoint Assumption (A_2) is equivalent to the triviality of a complex vector bundle over $\mathbb{T}^d$, namely the bundle of the null spaces of $1 - P_{\mathcal{I}}(k)$ for $k \in M^*$. In this geometrical perspective it is not difficult to see that Assumption (A_2) is always satisfied if either $d = 1$ or $\ell = 1$. Indeed, classification theory for bundles implies that any complex vector bundle over $\mathbb{T}^1 = S^1$ is trivial. As for $\ell = 1$, it is a classical result, due to Kostant and Weil, that smooth complex *line* bundles are completely classified by their first integer Chern class. In our case, the time-reversal symmetry of H_{per} implies the vanishing of the first integer Chern class, and therefore the triviality of the bundle. The same, and indeed slightly stronger, results can be proved with analytical techniques, as in [Nen$_3$] and references therein. By pushing forward the geometrical approach above, it is shown in [Pa] that Assumption (A_2) is generically satisfied for $d \leq 3$. ♢

Remark 5.10. In the presence of a strong external magnetic field the Bloch bands split into magnetic sub-bands. Generically, their first Chern number

does not vanish and therefore Assumption (A_2) fails. As well understood, the nonvanishing of the first Chern number is directly linked to the integer quantum Hall effect [TKNN, Si], hence our interest in extending Theorem 3 to magnetic Bloch bands. The required modifications of our theory will be discussed in [PST$_4$]. ♢

5.2 Adiabatic perturbation theory for Bloch bands

Let $P_n(k) = |\varphi_n(k)\rangle\langle\varphi_n(k)|$, then the projector on the n^{th} band subspace is given through $P_n = \int_{M^*}^{\oplus} \mathrm{d}k\, P_n(k)$. By construction the band subspaces are invariant under the dynamics generated by H_{per},

$$\left[\mathrm{e}^{-\mathrm{i}\mathcal{U}H_{\text{per}}\mathcal{U}^{-1}s}, P_n \right] = \left[\mathrm{e}^{-\mathrm{i}E_n(k)s}, P_n \right] = 0 \quad \text{for all } n \in \mathbb{N}\,,\ s \in \mathbb{R}\,.$$

Notice, however, that P_n is not a spectral subspace of H_{per}, in general. This is because in more than one space dimension it can happen that e.g. $E_n(k) < E_{n+1}(k)$ for all $k \in M^*$ but $\inf_k E_{n+1}(k) < \sup_k E_n(k)$.

According to the identity (5.11), in the original representation H_{per} acts on the n^{th} band subspace as

$$H_{\text{per}}\psi = \mathcal{U}^{-1}(E_n(k) \otimes \mathbf{1})\mathcal{U}\,\psi = E_n(-\mathrm{i}\nabla_x)\,\psi\,,$$

where $\psi \in \mathcal{U}^{-1}P_n\,\mathcal{U}\,L^2(\mathbb{R}^d)$. In other words, under the time evolution generated by the periodic Hamiltonian wave functions in the n^{th} band subspace propagate freely but with a modified dispersion relation given through the n^{th} band function $E_n(p)$.

In the presence of non-periodic external fields the subspaces $P_n\mathcal{H}$ are no longer invariant, since the external fields induce transitions between different band subspaces. If the potentials are varying slowly, these transitions are small and one expects that there still exist approximately invariant subspaces associated with isolated families of Bloch bands. The dynamics of states inside the decoupled subspaces should be generated by an effective Hamiltonian given through Peierls substitution.

In this section we apply the general scheme of adiabatic perturbation theory developed in Chapter 3 to the problem of perturbed Bloch bands in order to rigorously justify the heuristic picture.

We first present a theorem which summarizes the main results of this section. The remaining parts give the results and the proofs of the three main steps in space-adiabatic perturbation theory: In Section 5.2.1 we construct the almost invariant subspaces associated with isolated families of bands. In Section 5.2.2 we explain how to unitarily map the decoupled subspace to the reference Hilbert space. The effective Hamiltonian is constructed in Section 5.2.3 and we compute its asymptotic expansion explicitly including the subprincipal symbol. The main technical innovation necessary in order

to apply the scheme of Chapter 3 to the present case is the development of a pseudodifferential calculus for operators acting on sections of a bundle over the flat torus M^*, or, equivalently, acting on the space $\mathcal{H}_\tau$. This is done in Appendix B.

Before going into the details of the construction we present a theorem which encompasses the main results of this section. Generalizing from (5.9) it is convenient to introduce the following notation. For any separable Hilbert space $\mathcal{H}_\mathrm{f}$ and any unitary representation $\tau : \Gamma^* \to \mathcal{U}(\mathcal{H}_\mathrm{f})$, one defines the Hilbert space

$$L^2_\tau(\mathbb{R}^d, \mathcal{H}_\mathrm{f}) := \Big\{ \psi \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathcal{H}_\mathrm{f}) : \ \psi(k - \gamma^*) = \tau(\gamma^*)\, \psi(k) \Big\},$$

equipped with the inner product

$$\langle \psi,\, \varphi \rangle_{L^2_\tau} = \int_{M^*} \mathrm{d}k\, \langle \psi(k),\, \varphi(k) \rangle_{\mathcal{H}_\mathrm{f}}\,.$$

Using the results of the previous section and imposing Assumption (A_1), the Bloch-Floquet transform of the full Hamiltonian (5.5) is given through

$$H^\varepsilon_\mathrm{BF} := \mathcal{U}\, H^\varepsilon\, \mathcal{U}^{-1} = \frac{1}{2}\Big(-\mathrm{i}\nabla_y + k - A\big(\mathrm{i}\varepsilon\nabla^\tau_k\big)\Big)^2 + V_\Gamma(y) + \phi\big(\mathrm{i}\varepsilon\nabla^\tau_k\big) \quad (5.18)$$

with domain $L^2_\tau(\mathbb{R}^d, H^2(\mathbb{T}^d))$.

The application of space-adiabatic perturbation theory to an isolated family of bands $\{E_n(k)\}_{n\in\mathcal{I}}$ yields the following result, where the reference Hilbert space for the effective dynamics is $\mathcal{K} := L^2(\mathbb{T}^{d\,*}) \otimes \mathbb{C}^\ell$ with $\ell := \dim P_\mathcal{I}(k)$.

Theorem 5.11 (Peierls substitution and higher order corrections). *Let $\{E_n\}_{n\in\mathcal{I}}$ be an isolated family of bands, see Definition 5.7, and let Assumptions (A_1) and (A_2) be satisfied. Then there exist*

(i) *an orthogonal projection $\Pi^\varepsilon \in \mathcal{L}(\mathcal{H}_\tau)$,*
(ii) *a unitary map $U^\varepsilon \in \mathcal{L}(\Pi^\varepsilon \mathcal{H}_\tau, \mathcal{K})$, and*
(iii) *a self-adjoint operator $\widehat{h} \in \mathcal{L}(\mathcal{K})$*

such that

$$\big\| \big[\, H^\varepsilon_\mathrm{BF},\, \Pi^\varepsilon \,\big] \big\| = \mathcal{O}(\varepsilon^\infty)$$

and

$$\big\| \big(e^{-iH^\varepsilon_\mathrm{BF} t} - U^{\varepsilon\,*}\, e^{-i\widehat{h}t}\, U^\varepsilon\big)\Pi^\varepsilon \big\| = \mathcal{O}(\varepsilon^\infty(1 + |t|)).$$

The effective Hamiltonian $\widehat{h}$ is the Weyl quantization of a semiclassical symbol $h \in S^1_{\tau\equiv\mathbf{1}}(\varepsilon, \mathcal{L}(\mathbb{C}^\ell))$ with an asymptotic expansion which can be computed to any order. The $\mathcal{L}(\mathbb{C}^\ell)$-valued principal symbol $h_0(k,r)$ has matrix-elements

$$h_0(k,r)_{\alpha\beta} = \big\langle \psi_\alpha(k - A(r)), H_0(k,r)\, \psi_\beta(k - A(r)) \big\rangle\,, \quad (5.19)$$

where $\alpha, \beta \in \{1, \ldots, \ell\}$ and $H_0(k,r)$ is defined in (5.23).

The structure and the interpretation of the effective Hamiltonian are most transparent for the case of a single isolated band.

Corollary 5.12. *For an isolated ℓ-fold degenerate eigenvalue $E(k)$ the $\mathcal{L}(\mathbb{C}^\ell)$-valued symbol $h(k,r) = h_0(k,r) + \varepsilon h_1(k,r) + \mathcal{O}_0(\varepsilon^2)$ constructed in Theorem 5.11 has matrix-elements*

$$h_0(k,r)_{\alpha\beta} = \big(E(k - A(r)) + \phi(r)\big)\delta_{\alpha\beta} \tag{5.20}$$

and

$$\begin{aligned} h_1(k,r)_{\alpha\beta} &= \big(\nabla\phi(r) - \nabla E(\widetilde{k}) \times B(r)\big) \cdot \mathcal{A}(\widetilde{k})_{\alpha\beta} - B(r) \cdot M(\widetilde{k})_{\alpha\beta} \qquad (5.21) \\ &:= \Big(\partial_j\phi(r) - \partial_l E(\widetilde{k})\,\big(\partial_j A_l(r) - \partial_l A_j(r)\big)\Big)\,\mathcal{A}_j(\widetilde{k})_{\alpha\beta} \\ &\quad -\big(\partial_j A_l - \partial_l A_j\big)(r)\ \mathrm{Re}\left[\tfrac{\mathrm{i}}{2}\left\langle \partial_l\psi_\alpha(\widetilde{k}), (H_{\mathrm{per}} - E)(\widetilde{k})\ \partial_j\psi_\beta(\widetilde{k})\right\rangle_{\mathcal{H}_{\mathrm{f}}}\right], \end{aligned}$$

where summation over indices appearing twice is implicit, $\widetilde{k}(k,r) = k - A(r)$, and $\alpha, \beta \in \{1, \ldots, \ell\}$. The coefficients of the Berry connection are

$$\mathcal{A}(k)_{\alpha\beta} = \mathrm{i}\left\langle \psi_\alpha(k), \nabla\psi_\beta(k)\right\rangle_{\mathcal{H}_{\mathrm{f}}}. \tag{5.22}$$

In dimension $d = 3$ the subprincipal symbol (5.21) has a straight forward physical interpretation. The 2-forms B and M are naturally identified with the vectors $B = \mathrm{curl}A$ and

$$M(k)_{\alpha\beta} = \tfrac{\mathrm{i}}{2}\left\langle \nabla\psi_\alpha(k),\ \times(H_{\mathrm{per}}(k) - E(k))\nabla\psi_\beta(k)\right\rangle_{\mathcal{H}_{\mathrm{f}}}.$$

Then the symbol of the effective Hamiltonian has a form reminiscent of the one obtained from a multipole expansion for a classical charge distribution in weak external fields. In this sense one can interpret $\mathcal{A}(k)$ as an effective electric dipole moment and $M(k)$ as an effective magnetic dipole moment. We do not know if this analogy carries on to the higher order terms.

Remark 5.13. Our results hold for arbitrary dimension d. However, to simplify presentation, we use a notation motivated by the vector product and the duality between 1-forms and 2-forms for $d = 3$. If $d \neq 3$, then B, Ω_n and M_n are 2-forms. The inner product of 2-forms is

$$B \cdot M := *^{-1}(B \wedge *M) = \sum_{j=1}^{d}\sum_{i=1}^{d} B_{ij}M_{ij},$$

where $*$ denotes the Hodge duality induced by the euclidian metric, and for a vector field w and a 2-form F the "vector product" is

$$(w \times F)_j := (*^{-1}(w \wedge *F))_j = \sum_{i=1}^{d} w_i F_{ij},$$

where the duality between 1-forms and vector fields was used implicitly. $\diamondsuit$

Remark 5.14. E. I. Blount [Bl$_1$, Bl$_2$] derived the same effective Hamiltonian for isolated Bloch bands through a formal diagonalization of the full Hamiltonian in the Bloch-Floquet representation. It seems that his work remained largely unnoticed due to its complexity. ♢

Remark 5.15. The results of this chapter hold analogously when the external fields depend smoothly on time, cf. Remark 4.16. According to (4.44) the subprincipal symbol (5.21) of the effective Hamiltonian picks up an additional term

$$-\mathrm{i}\left\langle \psi_\alpha(k-A(r,t)), \partial_t \psi_\beta(k-A(r,t))\right\rangle = \dot{A}(r,t)\cdot \mathcal{A}(k-A(r,t))_{\alpha\beta}\,.$$

Hence $\dot{A}$ contributes, as expected, like an electric field to the Lorentz force in (5.21). ♢

Theorem 5.11 is a direct consequence of the results proved in Propositions 5.16, 5.18 and 5.19. The proof of Corollary 5.12 is given at the end of this section.

As explained before, the main idea of the proof is to adapt the general scheme of space-adiabatic perturbation theory to the case of the Bloch electron. While formally this seems straightforward, one must overcome two mathematical problems. First of all, in the present case the symbols are *unbounded*-operator-valued functions. One can deal with unbounded-operator-valued symbols by considering them as bounded operators from their domain equipped with the graph norm into the Hilbert space, cf. e.g. [DiSj].

The second, more serious problem consists in setting up a Weyl calculus for operators acting on spaces like $L^2_\tau(\mathbb{R}^d, \mathcal{H}_\mathrm{f})$. This is done in Appendix B and we will use in this section the terminology and notations introduced there.

The results of Appendix B allow us to write the Hamiltonian $H^\varepsilon_\mathrm{BF}$ as the Weyl quantization $H_0(k, \mathrm{i}\varepsilon\nabla_k)$ of the τ-equivariant symbol

$$H_0(k,r) = \frac{1}{2}\left(-\mathrm{i}\nabla_x + k - A(r)\right)^2 + V_\Gamma(x) + \phi(r) \tag{5.23}$$

acting on the Hilbert space $\mathcal{H}_\mathrm{f} := L^2(\mathbb{T}^d_x, \mathrm{d}\!\!^-x)$ with constant domain $\mathcal{D} := H^2(\mathbb{T}^d)$. For sake of clarity, we spend two more words on this point. For any fixed $(k,r) \in \mathbb{R}^{2d}$, $H_0(k,r)$ is regarded as a bounded operator from $\mathcal{D}$ to $\mathcal{H}_\mathrm{f}$ which is τ-equivariant with respect to the *bounded* representation $\tau_1 := \tau|_\mathcal{D}$ acting on $\mathcal{D}$ and the *unitary* representation $\tau_2 := \tau$ acting on $\mathcal{H}_\mathrm{f}$, cf. Definition B.2. Then the general theory developed in Appendix B can be applied: The usual Weyl quantization of H_0 is an operator from $\mathcal{S}'(\mathbb{R}^d, \mathcal{D})$ to $\mathcal{S}'(\mathbb{R}^d, \mathcal{H}_\mathrm{f})$ given by

$$\widehat{H}_0 = \frac{1}{2}\Big(-\mathrm{i}\nabla_y + k - A\big(\mathrm{i}\varepsilon\nabla_k\big)\Big)^2 + V_\Gamma(y) + \phi\big(\mathrm{i}\varepsilon\nabla_k\big)\,. \tag{5.24}$$

Then $\widehat{H}_0$ can be restricted to $L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathcal{D})$, since A and ϕ are smooth and bounded. Since H_0 is a τ-equivariant symbol, $\widehat{H}_0$ preserves τ-equivariance and can then be restricted to an operator from $L^2_\tau(\mathbb{R}^d, \mathcal{D})$ to $L^2_\tau(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}})$. To conclude that (5.24), restricted to $L^2_\tau(\mathbb{R}^d, \mathcal{D})$, agrees with (5.18), it is enough to recall that $\mathrm{i}\nabla^\tau_k$ is defined as $\mathrm{i}\nabla_k$ restricted to $H^1 \cap \mathcal{H}_\tau$ and to use the spectral calculus.

Moreover, if one introduces the order function $w(k, r) := (1 + k^2)$, then $H_0 \in S^w_\tau(\mathcal{L}(\mathcal{D}, \mathcal{H}))$. More generally, we will give the proofs for any symbol $H \in S^w_\tau(\varepsilon, \mathcal{L}(\mathcal{D}, \mathcal{H}))$, whose principal symbol is then denoted by H_0.

Warning: Note that in this chapter we use different symbol classes as compared to Chapter 3, namely those defined in terms order functions.

Otherwise we now proceed along the lines of the general scheme of Chapter 3. The basic strategy of the proof remains unchanged. However, since several important technical details are different, we give full proofs in the following instead of merely commenting on the changes.

5.2.1 The almost invariant subspace

In this section we construct the adiabatically decoupled subspace associated with an isolated family of bands. Given an isolated family of bands $\{E_n(k)\}_{n\in\mathcal{I}}$, we change notation and define $\pi_0(k, r) = P_{\mathcal{I}}(k - A(r))$. It follows from the τ-equivariance of H_0 and from the gap condition that $\pi_0 \in S^1_\tau(\mathcal{L}(\mathcal{H}_{\mathrm{f}}))$.

Proposition 5.16. *Let $\{E_n\}_{n\in\mathcal{I}}$ be an isolated family of bands and let Assumption (A_1) be satisfied. Then there exists an orthogonal projection $\Pi^\varepsilon \in \mathcal{L}(\mathcal{H}_\tau)$ such that*

$$\big[\, H^\varepsilon_{\mathrm{BF}},\, \Pi^\varepsilon \,\big] = \mathcal{O}_0(\varepsilon^\infty) \tag{5.25}$$

and $\Pi^\varepsilon = \widehat{\pi} + \mathcal{O}(\varepsilon^\infty)$, where $\widehat{\pi}$ is the Weyl quantization of a τ-equivariant semiclassical symbol

$$\pi \asymp \sum_{j\geq 0} \varepsilon^j \pi_j \quad \text{in} \quad S^1_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_{\mathrm{f}}))\,,$$

whose principal part $\pi_0(k, r)$ is the spectral projector of $H_0(k, r)$ corresponding to the given isolated family of bands.

We first construct π on a formal symbol level.

Lemma 5.17. *Let $w(k, r) = (1 + k^2)$. There exists a* unique *formal symbol*

$$\pi = \sum_{j=0}^{\infty} \varepsilon^j \pi_j \quad \in M^1_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_{\mathrm{f}})) \cap M^w_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_{\mathrm{f}}, \mathcal{D}))$$

such that $\pi_0(k, r) = P_{\mathcal{I}}\big(k - A(r)\big)$ and

(i) $\pi \sharp \pi = \pi$,
(ii) $\pi^* = \pi$,
(iii) $H \sharp \pi - \pi \sharp H = 0$.

Proof. We construct the formal symbol π locally in phase space and obtain by uniqueness, which can be proved as in Chapter 3, a globally defined formal symbol.

Fix a point $z_0 = (k_0, r_0) \in \mathbb{R}^{2d}$. From the continuity of the map $z \mapsto H(z)$ and the gap condition it follows that there exists a neighborhood $\mathcal{U}_{z_0}$ of z_0 such that for every $z \in \mathcal{U}_{z_0}$ the set $\{E_n(z)\}_{n\in\mathcal{I}}$ can be enclosed by a positively-oriented circle $\Lambda(z_0) \subset \mathbb{C}$ independent of z in such a way that $\Lambda(z_0)$ is symmetric with respect to the real axis,

$$\operatorname{dist}\big(\Lambda(z_0), \sigma(H(z))\big) \geq \frac{1}{4} C_{\mathrm{g}} \quad \text{for all} \quad z \in \mathcal{U}_{z_0} \tag{5.26}$$

and

$$\operatorname{Radius}(\Lambda(z_0)) \leq C_{\mathrm{r}}\,. \tag{5.27}$$

The constant C_{g} appearing in (5.26) is the same as in Definition 5.7 and the existence of a constant C_{r} independent of z_0 such that (5.27) is satisfied follows from the periodicity of $\{E_n(z)\}_{n\in\mathcal{I}}$ and the fact that A and ϕ are bounded. Indeed, Λ can be chosen Γ^*-periodic, i.e. such that $\Lambda(k_0+\gamma^*, r_0) = \Lambda(k_0, r_0)$ for all $\gamma^* \in \Gamma^*$.

Let us choose any $\zeta \in \Lambda(z_0)$ and restrict all the following expressions to $z \in \mathcal{U}_{z_0}$. We will construct a formal symbol $R(\zeta)$ with values in $\mathcal{L}(\mathcal{H}_{\mathrm{f}}, \mathcal{D})$ — the local Moyal resolvent of H — such that

$$(H - \zeta) \sharp R(\zeta) = \mathbf{1}_{\mathcal{H}_{\mathrm{f}}} \quad \text{and} \quad R(\zeta) \sharp (H - \zeta) = \mathbf{1}_{\mathcal{D}} \quad \text{on } \mathcal{U}_{z_0}\,. \tag{5.28}$$

To this end let

$$R_0(\zeta) = (H - \zeta)^{-1}\,,$$

where according to (5.26) $R_0(\zeta)(z) \in \mathcal{L}(\mathcal{H}_{\mathrm{f}}, \mathcal{D})$ for all $z \in \mathcal{U}_{z_0}$, and, using differentiability of $H(z)$, $\partial_z^\alpha R_0(\zeta)(z) \in \mathcal{L}(\mathcal{H}_{\mathrm{f}}, \mathcal{D})$ for all $z \in \mathcal{U}_{z_0}$. By construction one has

$$(H - \zeta) \sharp R_0(\zeta) = \mathbf{1}_{\mathcal{H}_{\mathrm{f}}} + \mathcal{O}_0(\varepsilon)\,,$$

where the remainder is $\mathcal{O}(\varepsilon)$ in the $\mathcal{L}(\mathcal{H}_{\mathrm{f}})$-norm. We proceed by induction. Suppose that

$$R^{(n)}(\zeta) = \sum_{j=0}^{n} \varepsilon^j R_j(\zeta)$$

with $R_j(\zeta)(z) \in \mathcal{L}(\mathcal{H}_{\mathrm{f}}, \mathcal{D})$ for all $z \in \mathcal{U}_{z_0}$ satisfies the first equality in (5.28) up to $\mathcal{O}(\varepsilon^{n+1})$, i.e.

$$(H - \zeta) \sharp R^{(n)}(\zeta) = \mathbf{1}_{\mathcal{H}_{\mathrm{f}}} + \varepsilon^{n+1} E_{n+1}(\zeta) + \mathcal{O}_0(\varepsilon^{n+2})\,, \tag{5.29}$$

where $E_{n+1}(\zeta)(z) \in \mathcal{L}(\mathcal{H}_\mathrm{f})$. By choosing

$$R_{n+1}(\zeta) = -R_0(\zeta)\, E_{n+1} \tag{5.30}$$

we obtain that $R^{(n+1)}(\zeta) = R^{(n)}(\zeta) + \varepsilon^{n+1} R_{n+1}(\zeta)$ takes values in $\mathcal{L}(\mathcal{H}_\mathrm{f}, \mathcal{D})$ and satisfies the first equality in (5.28) up to $\mathcal{O}(\varepsilon^{n+2})$. Hence the formal symbol $R(\zeta) = \sum_{j=0}^{\infty} \varepsilon^j R_j(\zeta)$ constructed that way satisfies the first equality in (5.28) exactly. By the same argument one shows that there exists a formal symbol $\widetilde{R}(\zeta)$ with values in $\mathcal{L}(\mathcal{H}_\mathrm{f}, \mathcal{D})$ which exactly satisfies the second equality in (5.28). By the associativity of the Moyal product, they must agree:

$$\widetilde{R}(\zeta) = \widetilde{R}(\zeta) \sharp (H - \zeta) \sharp R(\zeta) = R(\zeta) \qquad \text{on } \mathcal{U}_{z_0}.$$

Equations (5.28) imply that $R(\zeta)$ satisfies the resolvent equation

$$R(\zeta) - R(\zeta') = (\zeta - \zeta')\, R(\zeta) \sharp R(\zeta') \quad \text{on } \mathcal{U}_{z_0} \tag{5.31}$$

for any $\zeta, \zeta' \in \Lambda(z_0)$. From the resolvent equation it follows as in [PST$_1$] that the $\mathcal{L}(\mathcal{H}_\mathrm{f}, \mathcal{D})$-valued formal symbol $\pi = \sum_{j=0}^{\infty} \varepsilon^j \pi_j$ defined through

$$\pi_j(z) := \frac{\mathrm{i}}{2\pi} \oint_{\Lambda(z_0)} \mathrm{d}\zeta\, R_j(\zeta, z) \quad \text{on } \mathcal{U}_{z_0} \tag{5.32}$$

satisfies (i) and (ii) of Lemma 5.17. As for (iii) a little bit of care is required. Let $J : \mathcal{D} \to \mathcal{H}_\mathrm{f}$ be the continuous injection of $\mathcal{D}$ into $\mathcal{H}_\mathrm{f}$. Using (5.32) and (5.31) it follows that $\pi\, J \sharp R(\zeta) = R(\zeta)\, J \sharp \pi$ for all $\zeta \in \Lambda(z_0)$. Moyal-multiplying from left and from the right with $H - \zeta$ one finds $H \sharp \pi\, J = J\, \pi \sharp H$ as operators in $\mathcal{L}(\mathcal{D}, \mathcal{H}_\mathrm{f})$. However, by construction $H \sharp \pi$ takes values in $\mathcal{L}(\mathcal{H}_\mathrm{f})$ and, by density of $\mathcal{D}$, the same must be true for $\pi \sharp H$.

We are left to show that $\pi \in M^1_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_\mathrm{f})) \cap M^w_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_\mathrm{f}, \mathcal{D}))$. To this end notice that by construction π inherits the τ-equivariance of H, i.e.

$$\pi_j(k - \gamma^*, q) = \tau(\gamma^*)\, \pi_j(k, q)\, \tau(\gamma^*)^{-1}\,.$$

From (5.32) and (5.27) we conclude that for each $\alpha \in \mathbb{N}^{2d}$ and $j \in \mathbb{N}$ one has

$$\|(\partial_z^\alpha \pi_j)(z)\| \leq 2\pi C_\mathrm{r} \sup_{\zeta \in \Lambda(z_0)} \|(\partial_z^\alpha R_j)(\zeta, z)\|\,, \tag{5.33}$$

where $\|\cdot\|$ stands either for the norm of $\mathcal{L}(\mathcal{H}_\mathrm{f})$ or for the norm of $\mathcal{L}(\mathcal{H}_\mathrm{f}, \mathcal{D})$. In order to show that $\pi \in M^1_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_\mathrm{f}))$ it suffices to consider $z = (k, r) \in M^* \times \mathbb{R}^d$ since $\tau(\gamma^*)$ is unitary and thus the $\mathcal{L}(\mathcal{H}_\mathrm{f})$-norm of π is periodic. According to (5.33) we must show that

$$\|(\partial_z^\alpha R_j)(\zeta, z)\|_{\mathcal{L}(\mathcal{H}_\mathrm{f})} \leq C_{\alpha j} \quad \forall\, z \in \mathcal{U}_{z_0},\, \zeta \in \Lambda(z_0) \tag{5.34}$$

with $C_{\alpha j}$ independent of $z_0 \in M^* \times \mathbb{R}^d$.

We prove (5.34) by induction. Assume, by induction hypothesis, that for any $j \leq n$ one has that

$$R_j(\zeta) \in S^1_\tau(\mathcal{L}(\mathcal{H}_{\rm f})) \cap S^w_\tau(\mathcal{L}(\mathcal{H}_{\rm f}, \mathcal{D})) \tag{5.35}$$

uniformly in ζ, in the sense that the Fréchet semi-norms are bounded by ζ-independent constants. Then, according to Proposition B.4, $E_{n+1}(\zeta)$, as defined by (5.29), belongs to $S^{w^2}_\tau(\mathcal{L}(\mathcal{H}_{\rm f}))$ uniformly in ζ. By τ-equivariance, the norm of $E_{n+1}(\zeta)$ is periodic and one concludes that $E_{n+1}(\zeta) \in S^1_\tau(\mathcal{L}(\mathcal{H}_{\rm f}))$ uniformly in ζ. It follows from (5.30) that (5.35) is satisfied for $j = n+1$.

We are left to show that (5.35) is fulfilled for $j = 0$. We notice that according to (5.26) one has for all $z \in \mathbb{R}^{2d}$

$$\|R_0(\zeta)\|_{\mathcal{L}(\mathcal{H}_{\rm f})} = \|(H(z) - \zeta)^{-1}\|_{\mathcal{L}(\mathcal{H}_{\rm f})} = \frac{1}{\operatorname{dist}(\zeta, \sigma(H(z)))} \leq \frac{4}{C_{\rm g}}\,.$$

By the chain rule,

$$\|(\partial_z R_0)(\zeta, z)\|_{\mathcal{L}(\mathcal{H}_{\rm f})} = \|\big(R_0(\zeta)(\partial_z H_0) R_0(\zeta)\big)(z)\|_{\mathcal{L}(\mathcal{H}_{\rm f})}\,. \tag{5.36}$$

Since $\partial_z H_0\, R_0(\zeta)$ is a τ-equivariant $\mathcal{L}(\mathcal{H}_{\rm f})$-valued symbol, its norm is periodic. Therefore it suffices to estimate its norm for $z \in M^* \times \mathbb{R}^d$, which yields the required bound. For a general $\alpha \in \mathbb{N}^{2d}$, the norm of $\partial^\alpha_z R_0(\zeta)$ can be bounded in a similar way. This proves that $R_0(\zeta)$ belongs to $S^1_\tau(\mathcal{L}(\mathcal{H}_{\rm f}))$ uniformly in ζ.

On the other hand

$$\begin{aligned}
\|R_0(k,r)\|_{\mathcal{L}(\mathcal{H}_{\rm f},\mathcal{D})} &= \|(1+\Delta_x)\, R_0([k]+\gamma^*, r)\|_{\mathcal{L}(\mathcal{H}_{\rm f})} \\
&= \|(1+\Delta_x)\, \tau(\gamma^*) R_0([k], r) \tau^{-1}(\gamma^*)\|_{\mathcal{L}(\mathcal{H}_{\rm f})} \\
&\leq C\, \|(1+\gamma^{*2})(1+\Delta_x)\, R_0([k], r)\|_{\mathcal{L}(\mathcal{H}_{\rm f})} \\
&\leq C'(1+\gamma^{*2}) \leq 2C'(1+k^2)\,,
\end{aligned}$$

where we used the fact that $\|(1+\Delta_x)R_0(z)\|_{\mathcal{L}(\mathcal{H}_{\rm f})}$ is bounded for $z \in M^* \times \mathbb{R}^d$. The previous estimate and the fact that $\partial_z H_0\ R_0(\zeta) \in S^1_\tau(\mathcal{L}(\mathcal{H}_{\rm f}))$ yield

$$\begin{aligned}
\|(\partial_z R_0)(\zeta, z)\|_{\mathcal{L}(\mathcal{H}_{\rm f},\mathcal{D})} &= \|\big(R_0(\zeta)(\partial_z H_0) R_0(\zeta)\big)(z)\|_{\mathcal{L}(\mathcal{H}_{\rm f},\mathcal{D})} \\
&\leq C(1+k^2)\,.
\end{aligned}$$

Higher order derivatives, are bounded by the same argument, yielding that $R_0(\zeta)$ belongs to $S^w_\tau(\mathcal{L}(\mathcal{H}_{\rm f}, \mathcal{D}))$ uniformly in ζ. This concludes the induction argument.

From the previous argument it follows moreover that

$$\|(\partial^\alpha_z R_j)(\zeta, z)\|_{\mathcal{L}(\mathcal{H}_{\rm f},\mathcal{D})} \leq C_{\alpha j}\ w(z) \quad \forall\ z \in \mathcal{U}_{z_0},\ \zeta \in \Lambda(z_0) \tag{5.37}$$

with $C_{\alpha j}$ independent of $z_0 \in \mathbb{R}^{2d}$. By (5.33), this implies that $\pi \in M^w_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_{\rm f}, \mathcal{D}))$ and concludes the proof. □

Proof (of Proposition 5.16). From the projector constructed in Lemma 5.17 one obtains, by resummation, a semiclassical symbol $\pi \in S^1_\tau(\varepsilon, \mathcal{H}_\mathrm{f})$ whose asymptotic expansion is given by $\sum_{j\geq 0} \varepsilon^j \pi_j$. Then according to Proposition B.5 Weyl quantization yields a bounded operator $\widehat{\pi} \in \mathcal{L}(\mathcal{H}_\tau)$, which is approximately a projector in the sense that

$$\widehat{\pi}^2 = \widehat{\pi} + \mathcal{O}_0(\varepsilon^\infty) \text{ and } \widehat{\pi}^* = \widehat{\pi}\,.$$

We notice that Proposition B.4 implies that $H \widetilde{\sharp} \pi \in S^{w^2}_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_\mathrm{f}))$. But τ-equivariance implies that the norm is periodic and then $H \widetilde{\sharp} \pi$ belongs to $S^1_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_\mathrm{f}))$. Then $\pi \widetilde{\sharp} H = \left(H \widetilde{\sharp} \pi\right)^*$ belongs to the same class, so that $[H, \pi]_{\widetilde{\sharp}} \in S^1_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_\mathrm{f}))$. This *a priori* information on the symbol class, together with Lemma 5.17.(iii), assures that

$$[\widehat{H}, \widehat{\pi}] = \mathcal{O}_0(\varepsilon^\infty) \tag{5.38}$$

with the remainder bounded in the $\mathcal{L}(\mathcal{H}_\tau)$-norm.

In order to get a true projector, we proceed as in Section 3.1. For ε small enough, let

$$\Pi^\varepsilon := \frac{\mathrm{i}}{2\pi} \int_{|\zeta - 1| = \frac{1}{2}} \mathrm{d}\zeta \, (\widehat{\pi} - \zeta)^{-1}\,. \tag{5.39}$$

Then it follows as in Section 3.1 that ${\Pi^\varepsilon}^2 = \Pi^\varepsilon$, $\Pi^\varepsilon = \widehat{\pi} + \mathcal{O}_0(\varepsilon^\infty)$ and

$$\| \, [\widehat{H}, \Pi^\varepsilon] \, \|_{\mathcal{L}(\mathcal{H}_\tau)} \leq C \| \, [\widehat{H}, \widehat{\pi}] \, \|_{\mathcal{L}(\mathcal{H}_\tau)} = \mathcal{O}(\varepsilon^\infty)\,.$$

□

5.2.2 The intertwining unitaries

After we determined the decoupled subspace associated with an isolated family of bands, we aim at an effective description of the dynamics inside this subspace. In order to get a nice and workable formulation of the effective dynamics, it is convenient to map the decoupled subspace to a simpler reference space. The natural reference Hilbert space for the effective dynamics is $\mathcal{K} := L^2(\mathbb{T}^{d\,*}) \otimes \mathbb{C}^\ell$ with $\ell := \dim P_\mathcal{I}(k)$. Notation will be simpler in the following, if we think of the fibre $\mathbb{C}^\ell$ as a subspace of $\mathcal{H}_\mathrm{f}$. In order to construct such a unitary mapping, we reformulate Assumption (A_2) to get the analogue of (3.17) in the general setting.

Assumption $(\mathbf{A}_2')$. *Let $\{E_n(k)\}_{n\in\mathcal{I}}$ be an isolated family of bands and let $\pi_\mathrm{r} \in \mathcal{L}(\mathcal{H}_\mathrm{f})$ be an orthogonal projector with $\dim \pi_\mathrm{r} = \ell$. There is a unitary-operator-valued map $u_0 : \mathbb{R}^{2d} \to \mathcal{U}(\mathcal{H}_\mathrm{f})$ so that*

$$u_0(k,r)\, \pi_0(k,r)\, u_0^*(k,r) = \pi_\mathrm{r} \tag{5.40}$$

for any $(k,r) \in \mathbb{R}^{2d}$,

$$u_0(k+\gamma^*,r) = u_0(k,r)\tau(\gamma^*)^{-1}\,, \tag{5.41}$$

and u_0 *belongs to* $S^1(\mathcal{L}(\mathcal{H}_{\rm f}))$. ♢

Clearly,

$$u_0^*(k+\gamma^*,r) = \tau(\gamma^*)u_0^*(k,r). \tag{5.42}$$

An operator-valued symbol satisfying (5.42) (resp. (5.41)) is called left τ-covariant (resp. right τ-covariant).

The equivalence of (A_2) and (A_2') can be seen as follows. According to Assumption (A_2), there exists an orthonormal basis $\{\psi_j(k)\}_{j=1}^{\ell}$ of $\mathrm{Ran}P_{\mathcal{I}}(k)$ which is smooth and τ-equivariant with respect to k. Let $\pi_{\rm r} := \pi_0(k_0,r_0)$ for any fixed point (k_0,r_0). By the gap condition, $\dim\pi_{\rm r} = \dim P_{\mathcal{I}}(k)$. Then for any orthonormal basis $\{\chi_j\}_{j=1}^{\ell}$ for $\mathrm{Ran}\pi_{\rm r}$, the formula

$$\widetilde{u}_0(k,r) := \sum_{j=1}^{\ell} |\chi_j\rangle\,\langle\psi_j(k-A(r))| \tag{5.43}$$

defines a partial isometry which can be extended to a unitary operator $u_0(k,r) \in \mathcal{U}(\mathcal{H}_{\rm f})$. The fact that $\{\psi_j(k)\}_{j=1}^{\ell}$ spans $\mathrm{Ran}P_{\mathcal{I}}(k)$ implies (5.40), and the τ-equivariance of $\psi_j(k)$ reflects in (5.41).

Viceversa, given u_0 fulfilling Assumption (A_2'), one can check that the formula

$$\psi_j(k-A(r)) := u_0^*(k,r)\chi_j,$$

with $\{\chi_j\}_{j=1}^{\ell}$ spanning $\mathrm{Ran}\pi_{\rm r}$, defines an orthonormal basis for $\mathrm{Ran}P_{\mathcal{I}}(k)$ which satisfies Assumption (A_2).

After these remarks recall that the goal of this section is to construct a unitary operator which allow us to map the intraband dynamics from $\mathrm{Ran}\Pi^{\varepsilon}$ to an ε-independent reference space $\mathcal{K} \subset \mathcal{H}_{\rm ref}$. Since all the twisting of $\mathcal{H}_{\tau}$ has been absorbed in the τ-equivariant basis $\{\psi_j\}_{j=1}^{\ell}$, or equivalently in u_0, the space $\mathcal{H}_{\rm ref}$ can be chosen to be a space of *periodic* vector-valued functions, i.e.

$$\mathcal{H}_{\rm ref} := L^2_{\tau=\mathbf{1}}(\mathbb{R}^d,\mathcal{H}_{\rm f}) \cong L^2(\mathbb{T}^{d\,*},\mathcal{H}_{\rm f}).$$

As in Chapter 3 we introduce the orthogonal projector $\Pi_{\rm r} := \hat{\pi}_{\rm r} \in \mathcal{L}(\mathcal{H}_{\rm ref})$ since the effective intraband dynamics can be described in

$$\mathcal{K} := \mathrm{Ran}\Pi_{\rm r} \cong L^2_{\tau=\mathbf{1}}(\mathbb{R}^d,\mathbb{C}^{\ell}) \cong L^2(\mathbb{T}^{d\,*},\mathbb{C}^{\ell})$$

as it will become apparent later on. Recall that $\ell = \dim P_{\mathcal{I}}(k) = \dim\pi_{\rm r}$and that Assumption ($A_2$) and therefor also Assumption (A_2') is automatically satisfied, whenever $d \le 3$ or $|\mathcal{I}| = 1$.

Proposition 5.18. *Let* $\{E_n\}_{n\in\mathcal{I}}$ *be an isolated family of bands and let Assumptions* (A_1) *and* (A_2') *be satisfied. Then there exists a unitary operator* $U^{\varepsilon} : \mathcal{H}_{\tau} \to \mathcal{H}_{\rm ref}$ *such that*

$$U^\varepsilon \, \Pi^\varepsilon \, U^{\varepsilon\,*} = \Pi_{\rm r} \tag{5.44}$$

and $U^\varepsilon = \hat{u} + \mathcal{O}_0(\varepsilon^\infty)$*, where* $u \asymp \sum_{j\geq 0} \varepsilon^j u_j$ *belong to* $S^1(\varepsilon, \mathcal{L}(\mathcal{H}_{\rm f}))$*, is right* τ*-covariant at any order and has principal symbol* u_0*.*

Proof. By using the same argument as in Lemma 3.15 , one constructs first the formal symbol $\sum_{j\geq 0} \varepsilon^j u_j$. Since u_0 is right τ-covariant, one proves by induction that the same holds true for any u_j. Indeed, by referring to the notation of Section 3.2, one has that

$$u_{n+1} = (a_{n+1} + b_{n+1}) u_0$$

with $a_{n+1} = -\frac{1}{2} A_{n+1}$ and $b_{n+1} = [\pi_r, B_{n+1}]$. From the defining equation

$$u^{(n)} \sharp \, u^{(n)*} - 1 = \varepsilon^{n+1} A_{n+1} + \mathcal{O}(\varepsilon^{n+2})$$

and the induction hypothesis, it follows that A_{n+1} is a periodic symbol. Then $w^{(n)} := u^{(n)} + \varepsilon^{n+1} a_{n+1} u_0$ is right τ-covariant. Then the defining equation

$$w^{(n)} \sharp \, \pi \sharp \, w^{(n)*} - \pi_{\rm r} = \varepsilon^{n+1} B_{n+1} + \mathcal{O}(\varepsilon^{n+2})$$

shows that B_{n+1} is a periodic symbol, and so is b_{n+1}. Hence u_j is right τ-covariant, and there exists a semiclassical symbol $u \asymp \sum_j \varepsilon^j u_j$ so that $u \in S^1(\varepsilon, \mathcal{L}(\mathcal{H}_{\rm f}))$.

One notices that right τ-covariance is nothing but a special case of (τ_1, τ_2)-equivariance, for $\tau_2 \equiv \mathbf{1}$ and $\tau_1 = \tau$. Thus it follows from Proposition B.5 that the Weyl quantization of u is a bounded operator $\widehat{u} \in \mathcal{L}(\mathcal{H}_\tau, \mathcal{H}_{\rm ref})$ such that:

(i) $\widehat{u}\,\widehat{u}^* = \mathbf{1}_{\mathcal{H}_{\rm ref}} + \mathcal{O}_0(\varepsilon^\infty)$ and $\widehat{u}^*\widehat{u} = \mathbf{1}_{\mathcal{H}_\tau} + \mathcal{O}_0(\varepsilon^\infty)$,
(ii) $\widehat{u}\,\Pi^\varepsilon\,\widehat{u}^* = \Pi_{\rm r} + \mathcal{O}_0(\varepsilon^\infty)$.

Finally we modify $\widehat{u}$ as in Section 3.2 by an $\mathcal{O}_0(\varepsilon^\infty)$-term in order to get the unitary operator $U^\varepsilon \in \mathcal{U}(\mathcal{H}_\tau, \mathcal{H}_{\rm ref})$. □

5.2.3 The effective Hamiltonian

The final step in space-adiabatic perturbation theory is to compute the effective Hamiltonian for the intra-band dynamics. This is done, in principle, by projecting the full Hamiltonian $H^\varepsilon_{\rm BF}$ to the decoupled subspace and afterwards rotating to the reference space.

Proposition 5.19. *Let* $\{E_n\}_{n\in\mathcal{I}}$ *be an isolated family of bands and assume* (A_1) *and* (A_2)*. Let* h *be a resummation in* $S^1_{\tau\equiv\mathbf{1}}(\varepsilon, \mathcal{L}(\mathcal{H}_{\rm f}))$ *of the formal symbol*

$$h = u \sharp \pi \sharp H \sharp \pi \sharp u^* \, \in \, M^1_{\tau\equiv\mathbf{1}}(\varepsilon, \mathcal{L}(\mathcal{H}_{\rm f}))\,. \tag{5.45}$$

Then $\widehat{h} \in \mathcal{L}(\mathcal{H}_{\rm ref})$*,* $[\widehat{h}, \Pi_{\rm r}] = 0$ *and*

$$\big(\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm BF} t} - U^{\varepsilon\,*}\,\mathrm{e}^{-\mathrm{i}\widehat{h}t}\,U^\varepsilon\big)\Pi^\varepsilon = \mathcal{O}_0(\varepsilon^\infty(1+|t|))\,. \tag{5.46}$$

Proof. In the proof we denote $H^\varepsilon_{\mathrm{BF}}$ as $\widehat{H}$ to emphasize the fact that it is the Weyl quantization of $H \in S^w_\tau(\varepsilon, \mathcal{L}(\mathcal{D}, \mathcal{H}_{\mathrm{f}}))$.

First note that (5.45) follows from the following facts: according to Lemma 5.17 and Proposition B.4 we have that

$$\pi \sharp H \sharp \pi \in M^{w^2}_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_{\mathrm{f}})) = M^1_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_{\mathrm{f}}))\,,$$

where we used that τ is a unitary representation. With Proposition 5.18 it follows that $h \in M^1_{\tau\equiv 1}(\varepsilon, \mathcal{L}(\mathcal{H}_{\mathrm{f}}))$. Therefore $\widehat{h} \in \mathcal{L}(\mathcal{H}_{\mathrm{ref}})$ follows from Proposition B.5, while $[\widehat{h}, \Pi_{\mathrm{r}}] = 0$ is satisfied by construction.

It remains to check (5.46):

$$\begin{aligned}\big(\mathrm{e}^{-\mathrm{i}\widehat{H}t} - U^{\varepsilon\,*}\,\mathrm{e}^{-\mathrm{i}\widehat{h}t}\,U^\varepsilon\big)\Pi^\varepsilon &= \big(\mathrm{e}^{-\mathrm{i}\widehat{H}t} - \mathrm{e}^{-\mathrm{i}U^{\varepsilon\,*}\,\widehat{h}\,U^\varepsilon t}\big)\widehat{\pi} + \mathcal{O}_0(\varepsilon^\infty)\\ &= \big(\mathrm{e}^{-\mathrm{i}\widehat{\pi}\widehat{H}\widehat{\pi}t} - \mathrm{e}^{-\mathrm{i}U^{\varepsilon\,*}\,\widehat{h}\,U^\varepsilon t}\big)\widehat{\pi} + \mathcal{O}_0(\varepsilon^\infty)\\ &= \mathcal{O}(\varepsilon^\infty(1+|t|))\,,\end{aligned}$$

where the last equality follows from the usual Duhammel argument and the fact that the difference of the generators is $\mathcal{O}_0(\varepsilon^\infty)$ in the norm of bounded operators by construction. □

Since $[\widehat{h}, \Pi_{\mathrm{r}}] = 0$, the effective Hamiltonian will be regarded, without differences in notation, either as an element of $\mathcal{L}(\mathcal{H}_{\mathrm{ref}})$ or as an element of $\mathcal{L}(\mathcal{K})$.

We now compute the principal and the subprincipal symbol of $\widehat{h}$ for the special but most relevant case of an isolated ℓ-fold degenerate eigenvalue, i.e. $E_n(k) \equiv E(k)$ for every $n \in \mathcal{I}$, $|\mathcal{I}| = \ell$. Recall that in this special case Assumption (A_2) is equivalent to the existence of an orthonormal system of smooth and τ-equivariant Bloch functions corresponding to the eigenvalue $E(k)$. If $\ell = 1$ or $d \leq 3$, then Assumption (A_2) is always satisfied. The part of u_0 intertwining π_0 and π_{r} is given by Equation (5.43) where $\psi_j(k)$ are now Bloch functions, i.e. eigenvectors of $H_{\mathrm{per}}(k)$ to the eigenvalue $E(k)$.

Proof (of Corollary 5.12). In the following h is identified with $\pi_{\mathrm{r}} h \pi_{\mathrm{r}}$ and regarded as a $\mathcal{L}(\mathbb{C}^\ell)$-valued symbol. We consider the matrix elements

$$h(k,r)_{\alpha\beta} := \langle \chi_\alpha, h(k,r)\chi_\beta\rangle$$

for $\alpha, \beta \in \{1, \ldots, \ell\}$, where we recall that $\chi_\alpha = u_0(k,r)\psi_\alpha(k - A(r))$. Equation (5.20) follows immediately from the fact that $h_0 = u_0\, H_0\, u_0^*$ and that ψ_α are Bloch functions. As for h_1, we use the general formula (3.40), which reads applied to the present setting as

$$\begin{aligned}h_{1\,\alpha\beta}(k,r) = &-\mathrm{i}\,\big\langle \psi_\alpha(\widetilde{k}),\, \{E(\widetilde{k}) + \phi(r), \psi_\beta(\widetilde{k})\}\big\rangle\\ &- \tfrac{\mathrm{i}}{2}\big\langle \psi_\alpha(\widetilde{k}), \{(H_{\mathrm{per}}(\widetilde{k}) - E(\widetilde{k})), \psi_\beta(\widetilde{k})\}\big\rangle\,. \qquad (5.47)\end{aligned}$$

Here $\{A, \varphi\} = \nabla_r A \cdot \nabla_k \varphi - \nabla_k A \cdot \nabla_r \varphi$ are the Poisson brackets for an operator-valued function $A(k, r)$ acting on a vector-valued function $\varphi(k, r)$. We need to evaluate (5.47). Inserting (5.43) and performing a straightforward computation the first term in (5.47) gives the first term in (5.21) while the second term contributes to the $\alpha\beta$ matrix element with

$$\frac{\mathrm{i}}{2} \sum_{j,l=1}^{d} \big(\partial_j A_l - \partial_l A_j\big)(r) \left\langle \psi_\alpha(\widetilde{k}), \partial_l (H_{\mathrm{per}} - E)(\widetilde{k})\ \partial_j \psi_\beta(\widetilde{k}) \right\rangle_{\mathcal{H}_{\mathrm{f}}} .$$

The derivative on $(H_{\mathrm{per}} - E)$ can be moved to the first argument of the inner product by noticing that

$$0 = \nabla \big\langle \psi_\alpha, (H_{\mathrm{per}} - E)\phi \big\rangle = \big\langle \nabla \psi_\alpha, (H_{\mathrm{per}} - E)\phi \big\rangle + \big\langle \psi_\alpha, \nabla (H_{\mathrm{per}} - E)\phi \big\rangle$$

since ψ_α is in the kernel of $(H_{\mathrm{per}} - E)$. Finally the imaginary part of

$$\frac{\mathrm{i}}{2} \sum_{j,l=1}^{d} \big(\partial_j A_l - \partial_l A_j\big)(r) \left\langle \partial_l \psi_\alpha(\widetilde{k}),\ (H_{\mathrm{per}} - E)(\widetilde{k})\ \partial_j \psi_\beta(\widetilde{k}) \right\rangle_{\mathcal{H}_{\mathrm{f}}}$$

vanishes, as can be seen by direct computation, concluding the proof. □

5.3 Semiclassical dynamics for Bloch electrons

In Section 3.4.1 we discussed at length how to use the ε-independent classical flow generated by the principal symbol of the effective Hamiltonian in order to propagate semiclassical observables accurately to leading order in ε.

In this section we take a slightly different attitude and show how to incorporate the first order correction into the ε-dependent classical flow generated by the dynamical equations (5.4). The program is performed in two steps and it constitutes a slightly simpler version of the strategy presented in Section 4.1.3 for the Dirac equation. We first prove an Egorov theorem for observables in the reference representation and then, in order to obtain the result for the physical observables in Theorem 5.2, we translate the results from the reference representation on $\mathcal{H}_{\mathrm{ref}}$ back to the original representation on $L^2(\mathbb{R}^d)$.

Before performing this program, it is worthwhile to show that the semiclassical equations (5.4) are Hamiltonian equations with respect to a suitable symplectic structure. The Hamiltonian formulation has the advantage that the existence of global solutions of (5.4) follows immediately, and that it becomes straightforward to deal with questions related to symmetries and conserved quantities.

The dynamical equations (5.4), which define the ε-corrected semiclassical model, are given by

$$\begin{aligned} \dot{q} &= \nabla_\pi H_{\rm sc}(q,\pi) - \varepsilon\,\dot{\pi}\times\Omega_n(\pi)\,, \\ \dot{\pi} &= -\nabla_q H_{\rm sc}(q,\pi) + \dot{q}\times B(q) \end{aligned} \tag{5.48}$$

with Hamiltonian

$$H^\varepsilon_{\rm sc}(q,\pi) = E_n(\pi) + \phi(q) - \varepsilon\, M_n(\pi)\cdot B(q).$$

Recall that we are using the notation introduced in Remark 5.13 and that B and Ω_n are the 2-forms corresponding to the magnetic field and to the curvature of the Berry connection, i.e. in components

$$B(q)_{ij} = \big(\partial_i A_j - \partial_j A_i\big)(q)$$

for $i,j\in\{1,\dots,d\}$, and

$$\Omega_n(\pi)_{ij} = \big(\partial_i \mathcal{A}_j - \partial_j \mathcal{A}_i\big)(\pi)\,.$$

We fix the system of coordinates $z=(q,\pi)$ in $\mathbb{R}^{2d}$. The standard symplectic form $\Theta_0 = \Theta_0(z)_{lm}\,\mathrm{d}z_m\wedge\mathrm{d}z_l$, where $l,m\in\{1,\dots,2d\}$, has coefficients given by the constant matrix

$$\Theta_0(z) = \begin{pmatrix} 0 & -\mathbf{1}_{\mathbb{R}^d} \\ \mathbf{1}_{\mathbb{R}^d} & 0 \end{pmatrix}.$$

The symplectic form, which turns (5.48) into Hamilton's equation of motion for $H_{\rm sc}$, is given by the 2-form $\Theta_{B,\,\varepsilon} = \Theta_{B,\,\varepsilon}(z)_{lm}\,\mathrm{d}z_m\wedge\mathrm{d}z_l$ with coefficients

$$\Theta_{B,\,\varepsilon}(q,\pi) = \begin{pmatrix} B(q) & -\mathbf{1}_{\mathbb{R}^d} \\ \mathbf{1}_{\mathbb{R}^d} & \varepsilon\,\Omega_n(\pi) \end{pmatrix}. \tag{5.49}$$

For $\varepsilon = 0$ the 2-form $\Theta_{B,\,\varepsilon}$ coincides with the magnetic symplectic form Θ_B usually employed to describe in a gauge-invariant way the motion of a particle in a magnetic field ([MaRa], Section 6.6). For ε small enough, the matrix (5.49) defines a symplectic form, i.e. a closed non-degenerate 2-form. Indeed, since $\det\Theta_B = 1$ it follows that, for ε small enough, $\Theta_{B,\,\varepsilon}$ is not degenerate. In particular it is sufficient to choose

$$\varepsilon < \sup_{q,\pi\in\mathbb{R}^d} \big(\|B(q)\,\Omega_n(\pi)\| + \|\Omega_n(\pi)\|\big).$$

The closedness of $\Theta_{B,\,\varepsilon}$ follows from the fact that B and Ω_n correspond to closed 2-forms over $\mathbb{R}^d$.

With these definitions the corresponding Hamiltonian equations are

$$\Theta_{B,\,\varepsilon}(z)\;\dot{z} = \mathrm{d}H_{\rm sc}(z)\,,$$

or equivalently

$$\begin{pmatrix} B(q) & -\mathbf{1}_{\mathbb{R}^d} \\ \mathbf{1}_{\mathbb{R}^d} & \varepsilon\, \Omega_n(\pi) \end{pmatrix} \begin{pmatrix} \dot{q} \\ \dot{\pi} \end{pmatrix} = \begin{pmatrix} \nabla_q H(q,\pi) \\ \nabla_\pi H(q,\pi) \end{pmatrix},$$

which agrees with (5.48). We notice that our discussion remains valid if Ω_n admits a potential only locally, as it happens generically for magnetic Bloch bands.

We now turn to the derivation of the semiclassical model (5.4). Hence we assume that the isolated family of bands consists of a single non-degenerate Bloch band $E_n(k)$. We start with Egorov's theorem for observables in the reference space. As the only difference to the standard presentation of Egorov's theorem as in Section 3.4.1 we treat the first order corrections by considering an ε-dependent Hamiltonian flow instead of having a separate dynamics for the subprincipal symbol of an observable.

Proposition 5.20. *Let E_n be an isolated non-degenerate Bloch band and let $\widehat{h}$ be the effective Hamiltonian constructed in Theorem 5.11, which acts on the reference space $\mathcal{K} = L^2_{\tau\equiv 1}(\mathbb{R}^d)$ of Γ^*-periodic L^2_{loc}-functions. Let $\widetilde{\Phi}^t : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ be the Hamiltonian flow generated by the Hamiltonian function*

$$h_{\mathrm{cl}}(k,r) = h_0(k,r) + \varepsilon h_1(k,r)\,.$$

Then for any semiclassical observable $\widehat{a}$ with $a \in S^1(\varepsilon, \mathbb{C})$ we have that

$$\left\| \mathrm{e}^{\mathrm{i}\widehat{h}t/\varepsilon}\, \widehat{a}\, \mathrm{e}^{-\mathrm{i}\widehat{h}t/\varepsilon} \;-\; \widehat{a \circ \widetilde{\Phi}^t} \right\| = \mathcal{O}(\varepsilon^2) \tag{5.50}$$

uniformly for any finite interval in time.

Proof. Since the Hamiltonian function is bounded with bounded derivatives, it follows immediately that $a \circ \widetilde{\Phi}^t \in S^1(\varepsilon)$ and that $\frac{\mathrm{d}}{\mathrm{d}t}(a \circ \widetilde{\Phi}^t) \in S^1(\varepsilon)$. Therefore the proof is just the standard computation of Theorem 3.26

$$\begin{aligned} \mathrm{e}^{\mathrm{i}\widehat{h}t/\varepsilon}\, \widehat{a}\, \mathrm{e}^{-\mathrm{i}\widehat{h}t/\varepsilon} \;-\; \widehat{a \circ \widetilde{\Phi}^t} &= \int_0^t \mathrm{d}t'\, \frac{\mathrm{d}}{\mathrm{d}t'} \left(\mathrm{e}^{\mathrm{i}\widehat{h}t'/\varepsilon} \left(\widehat{a \circ \widetilde{\Phi}^{t-t'}} \right) \mathrm{e}^{-\mathrm{i}\widehat{h}t'/\varepsilon} \right) \\ &= \int_0^t \mathrm{d}t'\, \mathrm{e}^{\mathrm{i}\widehat{h}t'/\varepsilon} \left(\frac{\mathrm{i}}{\varepsilon} \left[\widehat{h}, \widehat{(a \circ \widetilde{\Phi}^{t-t'})} \right] - \widehat{\left(\tfrac{\mathrm{d}}{\mathrm{d}t'} (a \circ \widetilde{\Phi}^{t-t'}) \right)} \right) \mathrm{e}^{-\mathrm{i}\widehat{h}t'/\varepsilon}, \end{aligned}$$

together with the fact that the integrand is $\mathcal{O}(\varepsilon^2)$ in the norm of bounded operators, since by construction

$$\frac{\mathrm{d}}{\mathrm{d}t'} (a \circ \widetilde{\Phi}^{t-t'}) = \left\{ h_{\mathrm{cl}},\, a \circ \widetilde{\Phi}^{t-t'} \right\}$$

and, computing the expansion of the Moyal product according to Equation (A.11),

$$\frac{\mathrm{i}}{\varepsilon} \left[h, a \circ \widetilde{\Phi}^{t-t'} \right]_{\widetilde{\sharp}} = \left\{ h_{\mathrm{cl}},\, a \circ \widetilde{\Phi}^{t-t'} \right\} + \mathcal{O}(\varepsilon^2)\,.$$

□

In order to obtain the Egorov theorem for the physical observables, we need to undo the transformation to the reference space and the Bloch-Floquet transformation. We start with the simpler observation on how the Bloch-Floquet transformation maps semiclassical observables.

Proposition 5.21. *Let $a \in S^1(\varepsilon, \mathbb{C})$ be Γ^*-periodic, i.e. $a(q, p+\gamma^*) = a(q, p)$ for all $\gamma^* \in \Gamma^*$. Let $b(k, r) = a(r, k)$ then $b \in S^1_\tau(\varepsilon, \mathbb{C})$ and*

$$\widehat{a} = \mathcal{U}^* \widehat{b} \mathcal{U} \,,$$

where the Weyl quantization is in the sense of $\widehat{a} = a(\varepsilon x, -\mathrm{i}\nabla_x)$ acting on $L^2(\mathbb{R}^d)$ and $\widehat{b} = b(k, \varepsilon \mathrm{i}\nabla_k)$ acting on $\mathcal{H}_\tau$.

Remark 5.22. An analogous statement *cannot* be true for general operator-valued τ-equivariant symbols. For example, the symbol $b(k, r) := H_{\mathrm{per}}(k - A(r))$ is τ-equivariant and in particular a semiclassical observable. However, the corresponding operator in the original representation is

$$\mathcal{U}^* \widehat{b} \mathcal{U} = -\frac{1}{2}\big(-\mathrm{i}\nabla_x - A(\varepsilon x)\big)^2 + V_\Gamma(x)$$

which cannot be written as a ε-pseudodifferential operator with scalar symbol. ♢

Proof. We give the proof for $a(\cdot, p) \in \mathcal{S}(\mathbb{R}^d)$. The general result follows from standard density arguments, cf. [DiSj]. For $\psi \in \mathcal{S}(\mathbb{R}^d)$ we have according to (B.1) the explicit formula

$$\big(a(\varepsilon x, -\mathrm{i}\nabla_x)\psi\big)(x) = \frac{1}{(2\pi)^{d/2}} \sum_{\gamma \in \Gamma} \int_{\mathbb{R}^d} \mathrm{d}\eta \big(\mathcal{F}a\big)(\eta, \gamma)\ \mathrm{e}^{\mathrm{i}\varepsilon(\eta\cdot\gamma)/2} \mathrm{e}^{\mathrm{i}\varepsilon\eta\cdot x} \psi(x+\gamma)\,. \tag{5.51}$$

On the other hand for $(\mathcal{U}\psi)(k, r) =: \varphi(k, r)$ by definition it holds that

$$\big(b(k, \mathrm{i}\varepsilon\nabla_k)\varphi\big)(k, r) = \sum_{\gamma \in \Gamma} \int_{\mathbb{R}^d} \mathrm{d}\eta \big(\mathcal{F}b\big)(\gamma, \eta)\ \mathrm{e}^{-\mathrm{i}\varepsilon(\eta\cdot\gamma)/2} \mathrm{e}^{\mathrm{i}\gamma\cdot k} \varphi(k - \varepsilon\eta, r)\,. \tag{5.52}$$

The assumptions on a and ψ guarantee that all the integrals and sums in the following expressions are absolutely convergent and thus that interchanges in the order of integration are justified by Fubini's theorem.

We compute the inverse Bloch-Floquet transform of (5.52) using (5.10),

$$\begin{aligned} &\big(\mathcal{U}^{-1}\widehat{b}\,\varphi\big)(x) = \qquad\qquad (5.53)\\ &= \sum_{\gamma \in \Gamma} \int_{M^*} \mathrm{d}k \int_{\mathbb{R}^d} \mathrm{d}\eta \,\big(\mathcal{F}b\big)(\gamma, \eta)\ \mathrm{e}^{\mathrm{i}k\cdot x} \mathrm{e}^{-\mathrm{i}\varepsilon(\eta\cdot\gamma)/2} \mathrm{e}^{\mathrm{i}\gamma\cdot k} \varphi(k - \varepsilon\eta, [x])\\ &= \sum_{\gamma \in \Gamma} \int_{\mathbb{R}^d} \mathrm{d}\eta \,\big(\mathcal{F}b\big)(\gamma, \eta) \mathrm{e}^{\mathrm{i}\varepsilon(\eta\cdot\gamma)/2} \mathrm{e}^{\mathrm{i}\varepsilon\eta\cdot x} \int_{M^*} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}(k-\varepsilon\eta)\cdot(x+\gamma)} \varphi(k - \varepsilon\eta, [x])\,. \end{aligned}$$

The τ-equivariance of φ implies that the function $f(k,y) := \mathrm{e}^{\mathrm{i}k\cdot y}\varphi(k,[y])$ is exactly periodic in the first variable. Then the integral in $\mathrm{d}k$ can be shifted by an arbitrary amount, so that

$$\int_{M^*} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}(k-\varepsilon\eta)\cdot(x+\gamma)}\varphi(k-\varepsilon\eta,[x]) = \int_{M^*} \mathrm{d}k\, \mathrm{e}^{\mathrm{i}k\cdot(x+\gamma)}\varphi(k,[x+\gamma]) = \psi(x+\gamma)\,.$$

Inserting this expression in the last line of (5.53) and comparing with (5.51) concludes the proof. □

Before we arrive at the proof of Theorem 5.2, we must also understand how the unitary map constructed in Section 5.2.2 maps observables in the Bloch-Floquet representation to observables in the reference representation.

Proposition 5.23. *Let $b \in S^1(\varepsilon,\mathbb{C})$ be Γ^*-periodic in the first argument. Let $U^\varepsilon : \Pi_n^\varepsilon \mathcal{H}_\tau \to \mathcal{K}$ be the unitary map constructed in Section 5.2.2. Then*

$$U^\varepsilon\, \Pi_n^\varepsilon\, \widehat{b}\, \Pi_n^\varepsilon\, U^{\varepsilon\,*} = \widehat{c} + \mathcal{O}(\varepsilon^2)\,,$$

where $c(\varepsilon,k,r) = \big(b\circ T\big)(k,r)$ with

$$T : \mathbb{R}^{2d} \to \mathbb{R}^{2d}\,, \quad (k,r) \mapsto \Big(k + \varepsilon\, \mathcal{A}_m\big(k-A(r)\big)\nabla A_m(r),\; r + \varepsilon \mathcal{A}\big(k-A(r)\big)\Big)\,.$$

Here and in the following summation over indices appearing twice is implicitly assumed.

Proof. In order to compute $c = u \sharp \pi \sharp b \sharp \pi \sharp u^*$, observe that, since b is scalar-valued, the principal symbol remains unchanged, i.e. $c_0 = u_0\, \pi_0\, b_0\, \pi_0\, u_0^* = b_0$. For the subprincipal symbol we use the general transformation formula (3.40) obtained for the Hamiltonian, which applies to all operators whose principal symbol commutes with π_0. In this case the eigenvalue E in (3.40) must be replaced by the corresponding principal symbol. Hence we find that

$$\begin{aligned}
c_1(k,r) &= -\mathrm{i}\,\big\langle \psi(k-A(r)), \{b_0(k,r), \psi(k-A(r))\}\big\rangle \\
&\quad + \langle \psi(k-A(r)), b_1(k,r)\psi(k-A(r))\rangle \\
&= \partial_{k_n} b_0(k,r)\, \mathrm{i}\,\big\langle \psi(k-A(r)), \partial_m\psi(k-A(r))\big\rangle\, \partial_n A_m(r) \\
&\quad + \partial_{r_n} b_0(k,r)\, \mathrm{i}\,\big\langle \psi(k-A(r)), \partial_n\psi(k-A(r))\big\rangle + b_1(k,r) \\
&= \partial_{k_n} b_0(k,r)\, \mathcal{A}_m(k-A(r))\, \partial_n A_m(r) \\
&\quad + \partial_{r_n} b_0(k,r)\, \mathcal{A}_n(k-A(r)) + b_1(k,r)\,,
\end{aligned}$$

where summation over indices appearing twice is implicit. Now a comparison with the Taylor expansion of $\big(b\circ T\big)(k,r)$ in powers of ε proves the claim. □

We have now all the ingredients needed for the

Proof (of Theorem 5.2). Let $a \in C_{\mathrm{b}}^{\infty}(\mathbb{R}^{2d})$ be Γ^*-periodic in the second argument, then according to Proposition 5.21 we have

$$\Pi_n^\varepsilon \, \mathrm{e}^{\mathrm{i}H^\varepsilon t/\varepsilon} \, \widehat{a} \, \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} \, \Pi_n^\varepsilon = \mathcal{U}^* \, \Pi_n^\varepsilon \, \mathrm{e}^{\mathrm{i}H_{\mathrm{BF}}^\varepsilon t/\varepsilon} \, \widehat{b} \, \mathrm{e}^{-\mathrm{i}H_{\mathrm{BF}}^\varepsilon t/\varepsilon} \, \Pi_n^\varepsilon \, \mathcal{U} \tag{5.54}$$

with $b(k,r) = a(r,k)$. With Theorem 5.11 and Proposition 5.23 we find that

$$\Pi_n^\varepsilon \, \mathrm{e}^{\mathrm{i}H_{\mathrm{BF}}^\varepsilon t/\varepsilon} \, \widehat{b} \, \mathrm{e}^{-\mathrm{i}H_{\mathrm{BF}}^\varepsilon t/\varepsilon} \, \Pi_n^\varepsilon = U^{\varepsilon\,*} \, \mathrm{e}^{\mathrm{i}\widehat{\hbar} t/\varepsilon} \, \widehat{c} \, \mathrm{e}^{-\mathrm{i}\widehat{\hbar} t/\varepsilon} \, U^\varepsilon + \mathcal{O}(\varepsilon^2) \,, \tag{5.55}$$

where $c(\varepsilon,k,r) = \big(b \circ T\big)(k,r)$. Now we can apply Proposition 5.20 to conclude that

$$\mathrm{e}^{\mathrm{i}\widehat{\hbar} t/\varepsilon} \, \widehat{c} \, \mathrm{e}^{-\mathrm{i}\widehat{\hbar} t/\varepsilon} = \widehat{\big(c \circ \widetilde{\Phi}^t\big)} + \mathcal{O}(\varepsilon^2).$$

Since, for ε sufficiently small, T is a diffeomorphism, we can write

$$c \circ \widetilde{\Phi}^t = c \circ T^{-1} \circ T \circ \widetilde{\Phi}^t \circ T^{-1} \circ T =: c \circ T^{-1} \circ \overline{\Phi}^t \circ T = b \circ \overline{\Phi}^t \circ T \,,$$

where the flow $\overline{\Phi}_\varepsilon^t$ in the new coordinates will be computed explicitly below. Inserting the results into (5.55), we obtain

$$\begin{aligned} \Pi_n^\varepsilon \, \mathrm{e}^{\mathrm{i}H_{\mathrm{BF}}^\varepsilon t/\varepsilon} \, \widehat{b} \, \mathrm{e}^{-\mathrm{i}H_{\mathrm{BF}}^\varepsilon t/\varepsilon} \, \Pi_n^\varepsilon &= U^{\varepsilon\,*} \, \big(\widehat{b \circ \overline{\Phi}^t \circ T}\big) \, U^\varepsilon + \mathcal{O}(\varepsilon^2) \\ &= \Pi_n^\varepsilon \, \big(\widehat{b \circ \overline{\Phi}^t}\big) \, \Pi_n^\varepsilon + \mathcal{O}(\varepsilon^2) \,, \end{aligned}$$

where we used Proposition 5.23 for the second equality. Inserting into (5.54) we finally find that

$$\Pi_n^\varepsilon \, \mathrm{e}^{\mathrm{i}H^\varepsilon t/\varepsilon} \, \widehat{a} \, \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} \, \Pi_n^\varepsilon = \Pi_n^\varepsilon \, \big(\widehat{a \circ \overline{\Phi}^t}\big) \, \Pi_n^\varepsilon + \mathcal{O}(\varepsilon^2) \,, \tag{5.56}$$

where we did not make the exchange of the order of the arguments in a explicit.

Since we can compute the flow only approximately and only through its vector field, we make use of the following lemma.

Lemma 5.24. *Let $\Phi_i : \mathbb{R}^{2d} \times \mathbb{R} \to \mathbb{R}^{2d}$ be the flow associated with the vector field $v_i \in C_{\mathrm{b}}^{\infty}(\mathbb{R}^{2d}, \mathbb{R}^{2d})$, $i = 1, 2$.*

(i) *If for all $\alpha \in \mathbb{N}^{2d}$ there is a $c_\alpha < \infty$ such that*

$$\sup_{x \in \mathbb{R}^{2d}} |\, \partial^\alpha \, (v_1 - v_2)(x)| \leq c_\alpha \, \varepsilon^2 \,,$$

then for each bounded interval $I \subset \mathbb{R}$ there are constants $C_{I,\alpha} < \infty$ such that

$$\sup_{t \in I, x \in \mathbb{R}^{2d}} |\, \partial^\alpha \, (\Phi_1^t - \Phi_2^t)(x)| \leq C_{I,\alpha} \, \varepsilon^2 \,. \tag{5.57}$$

(ii) *Let $a \in S^1(\varepsilon, \mathbb{C})$. If (5.57) holds for the flows Φ_1, Φ_2, then there is a constant $C < \infty$, such that for all $t \in I$*

$$\big\| \widehat{a \circ \Phi_1^t} - \widehat{a \circ \Phi_2^t} \big\|_{\mathcal{L}(L^2(\mathbb{R}^d))} \leq C\, \varepsilon^2 \,.$$

Proof. Assertion (i) is just a simple application of Gronwall's lemma. Assertion (ii) follows from the fact that the norm of the quantization of a symbol in S^1 is bounded by a constant times the sup-norm of finitely many derivatives of the symbol, which are $\mathcal{O}(\varepsilon^2)$ according to (5.57). □

According to assertion (ii) of the lemma it suffices to show that

$$\overline{\Phi}^t(q,p) = \Big(\Phi^t_{n\,q}(q, p - A(q)),\, \Phi^t_{n\,\pi}(q, p - A(q)) + A(q) \Big) + \mathcal{O}(\varepsilon^2)$$

in the above sense, where Φ_n^t is the flow of (5.4). And from assertion (i) we infer that it suffices to prove the analogous properties on the level of the vector fields.

Through a subsequent change of coordinates we aim at computing the vector field of Φ_n^t up to an error of order $\mathcal{O}(\varepsilon^2)$. We start with the vector field of $\widetilde{\Phi}^t$. The effective Hamiltonian on the reference space including first order terms reads

$$\begin{aligned} h(r,k) &= E_n(k - A(r)) + \phi(r) \\ &\quad - \varepsilon \Big(F_{\mathrm{Lor}}(r, \nabla E_n(k - A(r))) \cdot \mathcal{A}(k - A(r)) + B(r) \cdot M(k - A(r)) \Big) \,, \end{aligned} \tag{5.58}$$

with the Lorentz force

$$F_{\mathrm{Lor}}(r, \nabla E_n(k - A(r))) = -\nabla\phi(r) + \nabla E_n(k - A(r)) \times B(r) \,.$$

To simplify the computation we switch to the kinetic momentum $\widetilde{k} = k - A(r)$. A straightforward computation, which is explained below, yields

$$\begin{aligned} \dot{r} &= \nabla E_n(\widetilde{k}) - \varepsilon \nabla_{\widetilde{k}} \Big(\mathcal{A}(\widetilde{k}) \cdot F_{\mathrm{Lor}}(r, \widetilde{k}) + B(r) \cdot M(\widetilde{k}) \Big) \,, \\ \dot{\widetilde{k}} &= -\nabla\phi(r) + \dot{r} \times B(r) + \varepsilon \nabla_r \Big(\mathcal{A}(\widetilde{k}) \cdot F_{\mathrm{Lor}}(r, \widetilde{k}) + B(r) \cdot M(\widetilde{k}) \Big) \,. \end{aligned} \tag{5.59}$$

As the next step we perform the change of coordinates induced by T,

$$q = r + \varepsilon \mathcal{A}(\widetilde{k}) \,, \qquad p = \widetilde{k} - A(r) + \varepsilon \nabla_r \big(\mathcal{A}(\widetilde{k}) \cdot A(r) \big) \,, \tag{5.60}$$

and then switch to the kinetic momentum

$$\begin{aligned} \pi = p - A(q) &= \widetilde{k} + \varepsilon \mathcal{A}_l(\widetilde{k}) \nabla A_l(r) - \varepsilon \mathcal{A}_l(\widetilde{k}) \partial_l A(r) + \mathcal{O}(\varepsilon^2) \\ &= \widetilde{k} + \varepsilon\, \mathcal{A}(\widetilde{k}) \times B(r) + \mathcal{O}(\varepsilon^2) \,, \end{aligned} \tag{5.61}$$

where we used Taylor expansion. The inverse transformations are

$$r = q - \varepsilon\, \mathcal{A}(\pi) + \mathcal{O}(\varepsilon^2) \quad \text{and} \quad \widetilde{k} = \pi - \varepsilon\, \mathcal{A}(\pi) \times B(q) + \mathcal{O}(\varepsilon^2)\,,$$

which, inserted into (5.59), yield (5.4).

This concludes our proof. However, since the corrected semiclassical equations (5.4) constitute a novel result, we supply the details of the computations skipped before. The canonical equations of motion of the Hamiltonian (5.58) are, componentwise,

$$\begin{aligned}
\dot{r}_j &= \partial_{k_j} h(r,k) = \partial_{k_j} E_n(k - A(r)) \\
&\quad -\varepsilon\, \partial_{k_j} \Big(F_{\mathrm{Lor}}(r, k - A(r)) \cdot \mathcal{A}(k - A(r)) + B(r) \cdot M(k - A(r)) \Big)\,,
\end{aligned}$$

$$\begin{aligned}
\dot{k}_j &= -\partial_{r_j} h(r,k) = -\partial_j \phi(r) + \partial_l E_n(k - A(r)) \partial_j A_l(r) \\
&\quad - \varepsilon\, \partial_{k_l} \Big(\mathcal{A}(k - A(r)) \cdot F_{\mathrm{Lor}}(r, k - A(r)) + B(r) \cdot M(k - A(r)) \Big)\, \partial_j A_l(r) \\
&\quad - \varepsilon\, \mathcal{A}_l(k - A(r)) \Big(\partial_j \partial_l \phi(r) - \big(\nabla E_n(k - A(r)) \times \partial_j B(r) \big)_l \Big) \\
&\quad + \varepsilon\, \partial_j B(r) \cdot M(k - A(r))\,,
\end{aligned}$$

with the convention to sum over repeated indices. Substituting $\widetilde{k} = k - A(r)$ one obtains

$$\dot{r}_j = \partial_j E_n(\widetilde{k}) - \varepsilon\, \partial_{\widetilde{k}_j} \Big(F_{\mathrm{Lor}}(r, \widetilde{k}) \cdot \mathcal{A}(\widetilde{k}) + B(r) \cdot M(\widetilde{k}) \Big)$$

and

$$\begin{aligned}
\dot{\widetilde{k}}_j &= \dot{k}_j - \partial_l A_j(r)\, \dot{r}_l \\
&= -\partial_j \phi(r) + \partial_l E_n(\widetilde{k})\, \partial_j A_l(r) \\
&\quad - \varepsilon\, \partial_{k_l} \Big(\mathcal{A}(\widetilde{k}) \cdot F_{\mathrm{Lor}}(r, \widetilde{k}) + M(\widetilde{k}) \cdot B(r) \Big)\, \partial_j A_l(r) \\
&\quad + \varepsilon\, \mathcal{A}_l(\widetilde{k})\, \partial_{r_j} F_{\mathrm{Lor}\, l}(r, \widetilde{k}) + \varepsilon\, \partial_j B(r) \cdot M(k - A(r)) - \partial_l A_j(r)\, \dot{r}_l \\
&= -\partial_j \phi(r) + \dot{r}_l \Big(\partial_j A_l(r) - \partial_l A_j(r) \Big) \\
&\quad + \varepsilon\, \mathcal{A}_l(\widetilde{k})\, \partial_{r_j} F_{\mathrm{Lor}\, l}(r, \widetilde{k}) + \varepsilon\, \partial_j B(r) \cdot M(\widetilde{k}) \\
&= -\partial_j \phi(r) + \big(\dot{r} \times B(r) \big)_j + \varepsilon\, \mathcal{A}_l(\widetilde{k})\, \partial_{r_j} F_{\mathrm{Lor}\, l}(r, \widetilde{k}) + \varepsilon\, \partial_j B(r) \cdot M(\widetilde{k})\,,
\end{aligned}$$

as claimed in (5.59).

Next we substitute (5.60) and (5.61). In the following computations we frequently use Taylor expansion to first order and drop terms of order ε^2 without notice. In particular in the terms of order ε one can replace r by q and $\widetilde{k}$ by π. We find that

$$\begin{aligned}
\dot{q}_j &= \dot{r}_j + \varepsilon\, \dot{\mathcal{A}}_j(\pi) \\
&= \partial_j E_n(\pi) - \varepsilon \Big(\mathcal{A}(\pi) \times B(q) \Big)_l\, \partial_l \partial_j E_n(\pi)
\end{aligned}$$

$$
\begin{aligned}
&- \varepsilon\, \partial_{\pi_j} \Big(\big(- \nabla\phi(q) + \nabla E_n(\pi) \times B(q) \big)_l \mathcal{A}_l(\pi) + B(q) \cdot M(\pi) \Big) \\
&+ \varepsilon \partial_l \mathcal{A}_j \dot{\pi}_l \\
&= \partial_j E_n(\pi) - \varepsilon \dot{\pi}_l \Big(\partial_j \mathcal{A}_l - \partial_l \mathcal{A}_j \Big) - \varepsilon\, B(q) \cdot \partial_j M(\pi) \\
&= \partial_j E_n(\pi) - \varepsilon \big(\dot{\pi} \times \Omega(\pi) \big)_j - \varepsilon\, B(q) \cdot \partial_j M(\pi)\,,
\end{aligned}
$$

where we used already that $\dot{\pi} = F_{\mathrm{Lor}} + \mathcal{O}(\varepsilon)$. Thus we obtained the first equation of (5.4). For the second equation we find

$$
\begin{aligned}
\dot{\pi}_j &= \dot{\tilde{k}}_j + \varepsilon \frac{\mathrm{d}}{\mathrm{d}t} \Big(\mathcal{A}(\pi) \times B(q) \Big) \\
&= - \partial_j \phi(q) + \varepsilon \mathcal{A}_l(\pi) \partial_l \partial_j \phi(q) \\
&\quad + \big(\dot{q} \times B(q) \big)_j - \varepsilon \big(\dot{\mathcal{A}}(\pi) \times B(q) \big)_j - \varepsilon \Big(\dot{q} \times \big(\mathcal{A}_l(\pi) \partial_l B(q) \big) \Big)_j \\
&\quad + \varepsilon\, \mathcal{A}_l(\pi) \partial_{q_j} F_{\mathrm{Lor}\, l}(q, \pi) + \varepsilon\, \partial_j B(q) \cdot M(\pi) \\
&\quad + \varepsilon \big(\dot{\mathcal{A}}(\pi) \times B(q) \big)_j + \varepsilon \Big(\mathcal{A}(\pi) \times \big(\dot{q}_l \partial_l B(q) \big) \Big)_j \\
&= - \partial_j \phi(q) + \big(\dot{q} \times B(q) \big)_j + \varepsilon\, \partial_j B(q) \cdot M(\pi)\,,
\end{aligned}
$$

where the fact that

$$
\varepsilon\, \mathcal{A}_\ell(\pi) \Big(\partial_{q_j} F_{\mathrm{Lor}\, l}(q, \pi) + \partial_l \partial_j \phi(q) \Big) = \varepsilon\, \mathcal{A}_l(\pi) \Big(\dot{q} \times \partial_j B(q) \Big)_l + \mathcal{O}(\varepsilon^2)
$$

cancels the remaining two terms is not so obvious, but can be checked by direct computation. □

6 Adiabatic decoupling without spectral gap

Until recently the gap condition in adiabatic theorems was assumed to be essential and irreplaceable. Following the proof of the standard first order time-adiabatic theorem of Section 2.1, one finds that the gap condition enters in two ways.

(i) It is needed in order to conclude from the regularity of the Hamiltonian $H(t)$ as a function of t on the regularity of the spectral projection $P_*(t)$ as a function of t, cf. the argument before Lemma 2.4.
(ii) To show that the difference of the full and the adiabatic time-evolution stays of order ε even for macroscopic times, this difference was written as the integral over an oscillating function. The minimal frequency of this function is proportional to the size of the gap. As a consequence the averaging argument over long times fails, whenever the gap closes.

In the present chapter we develop a time-adiabatic theorem and a space-adiabatic theorem without gap condition. Problem (i) in the above list is basically solved by assumption, i.e. in adiabatic theorems without gap condition the smoothness of the projections must be assumed. Problem (ii) is solved by a more careful analysis. The basic idea is very simple: In the presence of a spectral gap the reduced resolvent $R(E)\,(1-P_E) = (H-E)^{-1}\,(1-P_E)$ is a bounded operator. Here E is an eigenvalue of H and P_E the corresponding spectral projection. The standard proof of the adiabatic theorem as presented in Section 2.1 basically estimates the non-adiabatic transitions by $\varepsilon \sup_t \|R(E(t))\,(1-P_{E(t)})\| \leq \varepsilon C$. Without a spectral gap the reduced resolvent is not a bounded operator anymore, a failure which can be cured by moving into the complex plane and considering $R(E+\mathrm{i}\delta)$ instead. While for space-adiabatic theory without gap condition some assumptions about the limiting behavior of $R(E+\mathrm{i}\delta)$ as $\delta \to 0$ must be made, the following variant of a lemma due to Avron and Elgart [AvEl$_1$] can be used to prove a general time-adiabatic theorem without gap condition.

Lemma 6.1. *Let H be a self-adjoint operator on some Hilbert space $\mathcal{H}$. Let E be an eigenvalue of H with spectral projection P_E. Then for all $\psi \in \mathcal{H}$*

$$\lim_{\delta \to 0} \delta \,\| \,(H - E - \mathrm{i}\delta)^{-1}\,(\mathbf{1} - P_E)\,\psi \,\| = 0\,. \tag{6.1}$$

S. Teufel: LNM 1821, pp. 173–201, 2003.

Notice that this result is not completely obvious, since the simple norm estimate

$$\| (H - E - \mathrm{i}\delta)^{-1} (\mathbf{1} - P_E) \| \leq 1/\mathrm{dist}\big(E + \mathrm{i}\delta, \sigma(H(1 - P_E))\big) \leq 1/\delta$$

would not yield the desired convergence.

Proof (of Lemma 6.1). Let $\varphi = (\mathbf{1} - P_E)\psi$, then

$$\begin{aligned} \lim_{\delta \to 0} \|\delta\, R(E + \mathrm{i}\delta)\, (\mathbf{1} - P_E)\, \psi\|^2 &= \lim_{\delta \to 0} \| \,\delta R(E + \mathrm{i}\,\delta, t)\, \varphi\|^2 \qquad (6.2) \\ &= \lim_{\delta \to 0} \int_{\mathbb{R}} \mu_\varphi(\mathrm{d}\lambda) \frac{\delta^2}{(\lambda - E)^2 + \delta^2} = \mu_\varphi(E)\,, \end{aligned}$$

where μ_φ denotes the spectral measure of H for φ. Since $\varphi \in \mathrm{Ran}(\mathbf{1} - P_E)$ and P_E is the spectral projection corresponding to E, $\mu_\varphi(E) = 0$ follows. □

This lemma allows one to prove a time-adiabatic theorem without gap condition under very general assumptions. On the other hand, if one is interested in the rate of convergence of the adiabatic limit, better estimates for the reduced resolvent are needed, and, as we shall see, available in the main application discussed in Section 6.3.

While there is no qualitative difference between the time-adiabatic and the space-adiabatic theorems with gap condition, it turns out that this is no longer so in the presence of eigenvalue crossings, i.e. a particular case when the gap condition fails. The reason is, roughly speaking, that in the time-adiabatic case all states move through the crossing at the same fixed speed, while in the space-adiabatic setting some states might remain near the crossing for very long times. As a consequence *uniform* results require much stronger assumptions in the space-adiabatic setting than in the time-adiabatic setting. In particular, a countable number of eigenvalue crossings is allowed in the time-adiabatic theorem, Theorem 6.2. For further details we refer to Remark 6.5.

General time-adiabatic results without gap condition are only quite recent and were obtained independently by Bornemann [Bor] and by Avron and Elgart [AvEl$_1$]. The material of this chapter is taken from [Te$_1$] and [Te$_2$]. In [Te$_1$] the proof of [AvEl$_1$] is simplified considerably and at the same time the result is improved. The translation of the method to the space-adiabatic setting was first done in [Te$_2$].

6.1 Time-adiabatic theory without gap condition

Recall the Schrödinger equation with time dependent Hamiltonian

$$\mathrm{i}\varepsilon \frac{\mathrm{d}}{\mathrm{d}t} U^\varepsilon(t, t_0) = H(t)\, U^\varepsilon(t, t_0)\,, \quad U^\varepsilon(t_0, t_0) = \mathbf{1}\,. \qquad (6.3)$$

Here $H(t)$, $t \in J$ is a family of self-adjoint operators on some Hilbert space $\mathcal{H}$ with a common dense domain $\mathcal{D}$.

Let $U_{\mathrm{a}}^{\varepsilon}(t, t_0)$ denote again the adiabatic time evolution given as the solution of (6.3) with $H(t)$ replaced by $H_{\mathrm{a}}(t) := H(t) + \mathrm{i}\,\varepsilon\,[\dot{P}(t), P(t)]$. Recall that the adiabatic evolution exactly intertwines $P(t_0)$ and $P(t)$, i.e.

$$U_{\mathrm{a}}^{\varepsilon *}(t, t_0)\, P(t)\, U_{\mathrm{a}}^{\varepsilon}(t, t_0) = P(t_0)\,. \tag{6.4}$$

Theorem 6.2. *Let $H(\cdot)$ satisfy the assumptions of Proposition 2.1. Suppose that $E(t)$ is an eigenvalue of $H(t)$ and that $P(t)$ is a family of finite rank projections such that $H(t)P(t) = E(t)P(t)$ for all $t \in J$, $P(\cdot) \in C_{\mathrm{b}}^2(J, \mathcal{L}(\mathcal{H}))$ and such that $P(t)$ is the spectral projection of $H(t)$ on $\{E(t)\}$ for almost all $t \in J$. Then the solution $U^{\varepsilon}(t, t_0)$ of (6.3) satisfies for each bounded interval $J' \subseteq J$ and $t_0 \in J'$*

$$\lim_{\varepsilon \to 0} \sup_{t \in J'} \| U^{\varepsilon}(t, t_0) - U_{\mathrm{a}}^{\varepsilon}(t, t_0) \|_{\mathcal{L}(\mathcal{H})} = 0\,. \tag{6.5}$$

Note that if $E(t)$ crosses a different eigenvalue $E_1(t)$ at some time $t = t_0$, i.e. $E(t) = E_1(t)$ only for $t = t_0$, then the rank of the spectral projection $P_{\{E(t)\}}(H(t))$ jumps and thus it is not even continuous at $t = t_0$. If it is possible to continue $P_{\{E(t)\}}(H(t))$ through the crossing in a differentiable way, such a crossing (actually a countable number of them) is included in the above formulation of the theorem.

The proof of Theorem 6.2 will actually yield simple criteria for estimating the order of the error in (6.5). These criteria are basically assumptions on the rate of convergence in (6.1) for the reduced resolvent. We omit the corresponding discussion at this point and refer to [Te$_1$] and to Section 6.2, where the space-adiabatic theorem without gap condition will be presented with all details.

A different approach to the adiabatic theorem without gap condition is due to Bornemann [Bor]. His result was the motivation for relaxing the "spectrality" condition from $P(t) = P_{\{E(t)\}}(H(t))$ for all $t \in J$, as in [AvEl$_1$], to $P(t) = P_{\{E(t)\}}(H(t))$ for almost all $t \in J$, as in [Bor]. However, while his approach based on weak convergence arguments is quite flexible and elegant, it yields only the adiabatic decoupling of the subspace, i.e.

$$\lim_{\varepsilon \to 0} \sup_{t \in J'} \| (1 - P(t))\, U^{\varepsilon}(t, t_0)\, P(t_0) \|_{\mathcal{L}(\mathcal{H})} = 0\,, \tag{6.6}$$

but not the effective dynamics inside the subspace as in (6.5).

Proof (of Theorem 6.2). To simplify notation, we set without loss of generality $t_0 = 0$ and abbreviate $U^{\varepsilon}(t, 0)$ as $U^{\varepsilon}(t)$. Next note that the adiabatic propagator is well defined and leaves invariant $\mathcal{D}$, since $H_{\mathrm{a}}(t)$ satisfies the assumptions of Proposition 2.1. This is the reason for requiring $P(\cdot) \in C^2(J, \mathcal{L}(\mathcal{H}))$, as for the remainder of the proof $P(\cdot) \in C^1(J, \mathcal{L}(\mathcal{H}))$ would suffice, cf. [Te$_2$].

We proceed as in Chapter 2 and express the difference of the unitaries in terms of the difference of the generators,

$$\begin{aligned} \| U^\varepsilon(t) - U_{\rm a}^\varepsilon(t)\| &= \| \int_0^t {\rm d}t' \frac{\rm d}{{\rm d}t}\Big(U^{\varepsilon *}(t') U_{\rm a}^\varepsilon(t)\Big) \| \\ &= \| \int_0^t {\rm d}t'\, U^{\varepsilon *}(t') [\dot P(t'), P(t')] U_{\rm a}^\varepsilon(t') \| \,. \end{aligned} \tag{6.7}$$

If one can find bounded operators $X(t)$, $Y(t)$ satisfying

$$[\dot P(t), P(t)] = [H(t), X(t)] + Y(t)\,, \tag{6.8}$$

then the integrand in (6.7) can be written as a time derivative plus a remainder,

$$\begin{aligned} U^{\varepsilon *}[\dot P, P]\, U_{\rm a}^\varepsilon = -{\rm i}\,\varepsilon \frac{\rm d}{{\rm d}t}\Big(U^{\varepsilon *}\, X\, U^\varepsilon U^{\varepsilon *} U_{\rm a}^\varepsilon\Big) + {\rm i}\,\varepsilon \Big(U^{\varepsilon *}\, X [\dot P, P] U_{\rm a}^\varepsilon + U^{\varepsilon *} \dot X U_{\rm a}^\varepsilon\Big) \\ + U^{\varepsilon *}\, Y\, U_{\rm a}^\varepsilon \,, \end{aligned} \tag{6.9}$$

and (6.9) in (6.7) yields the bound

$$\begin{aligned} &\sup_{t\in J'} \| U^\varepsilon(t) - U_{\rm a}^\varepsilon(t)\| \leq \\ &\quad \varepsilon \sup_{t\in J'} 2(1 + \|\dot P(t)\|)\, \|X(t)\| + \int_0^t {\rm d}t' \, \Big(\varepsilon\, \|\dot X(t')\| + \|Y(t')\| \Big) \,. \end{aligned} \tag{6.10}$$

The proof as given in Section 2.1 corresponds to the choice

$$X_{\rm gap}(t) := R(E(t), t) \dot P(t) P(t) + P(t) \dot P(t) R(E(t), t)\,,$$

$$Y_{\rm gap}(t) \equiv 0\,.$$

Indeed, in the presence of a gap δ separating $E(t)$ from the rest of the spectrum of $H(t)$, $X_{\rm gap}(t)$, $Y_{\rm gap}(t)$ would be a solution of (6.8) with $X_{\rm gap}(\cdot) \in C^1(J', \mathcal{L})$. This is because

$$\dot P(t) = (1 - P(t))\, \dot P(t)\, P(t) + P(t)\, \dot P(t)\, (1 - P(t)) \tag{6.11}$$

and thus

$$\|R(E(t), t) \dot P(t) P(t)\| = \|R(E(t), t)(1 - P(t))\, \dot P(t)\, P(t)\| \leq \|\dot P(t)\|/\delta\,.$$

Hence, in the presence of a gap (6.10) gives the standard result of Section 2.1:

$$\sup_{t\in J'} \| U_{\rm a}^\varepsilon(t) - U^\varepsilon(t)\| = \mathcal{O}(\varepsilon)\,.$$

Instead of using a cutoff function $\widetilde g$ to define $R(E(t), t)\, \widetilde g((H(t) - E(t))/\delta)$ in absence of a gap as in [AvEl$_1$], we shift the resolvent into the complex plane and define

$$X_\delta(t) := R(E(t) - \mathrm{i}\,\delta, t)\,\dot{P}(t)\,P(t) \;+\; \text{adj.} \;=\; X_\delta(t)P(t) \;+\; \text{adj.}\,,$$
$$Y_\delta(t) := \mathrm{i}\,\delta R(E(t) - \mathrm{i}\,\delta, t)\,\dot{P}(t)\,P(t) \;-\; \text{adj.} \;=\; Y_\delta(t)P(t) \;-\; \text{adj.}\,.$$

Here again "$\pm$ adj." means that the adjoint of the first term in the sum is added resp. subtracted. With our definition the fact that $X_\delta(t)$ and $Y_\delta(t)$ solve (6.8) is obvious and the following bounds have elementary proofs even in the case of unbounded $H(t)$.

We will show that $X_\delta(\cdot), Y_\delta(\cdot) \in C^1_{\mathrm{b}}(J', \mathcal{L})$ for $\delta \in (0, 1]$ and that for some constant $C < \infty$

$$\sup_{t\in J'} \|X_\delta(t)\| \le \frac{C}{\delta}\,, \quad \sup_{t\in J'} \left\|\dot{X}_\delta(t)\right\| \le \frac{C}{\delta^2}\,, \quad \sup_{t\in J',\delta\in(0,1]} \|Y_\delta(t)\| < \infty \tag{6.12}$$

and

$$\|Y_\delta(t)\| \to 0 \quad \text{as} \quad \delta \to 0 \tag{6.13}$$

for almost all $t \in J'$. Then the theorem follows by inserting (6.12) and (6.13) into (6.10), using dominated convergence and choosing $\delta = \delta(\varepsilon)$ with $\lim_{\varepsilon\to 0} \delta(\varepsilon) = 0$ and $\lim_{\varepsilon\to 0} \delta^2(\varepsilon)/\varepsilon = \infty$.

It suffices to establish (6.12)–(6.13) for $X_\delta(t)P(t)$ resp. $Y_\delta(t)P(t)$, since the adjoints have the same norms. The first and the third bound in (6.12) follow from $\|R(E(t)-\mathrm{i}\,\delta, t)\| \le 1/\delta$ and from $P(\cdot) \in C^2_{\mathrm{b}}(J', \mathcal{L})$. For the second bound observe that

$$\frac{\mathrm{d}}{\mathrm{d}s} R(E(t) - \mathrm{i}\,\delta, t) = -R(E(t) - \mathrm{i}\,\delta, t)(\dot{H}(t) - \dot{E}(t))R(E(t) - \mathrm{i}\,\delta, t)$$

and thus, by inserting $\mathbf{1} = R(\mathrm{i}, t)\,(H(t) - (E(t) - \mathrm{i}\,\delta) - \mathrm{i} + (E(t) - \mathrm{i}\,\delta))$,

$$\|\dot{R}(E(t) - \mathrm{i}\,\delta, t)\| \le \left(\frac{\|\dot{H}(t)R(\mathrm{i}, t)\|(2\delta + 1 + |E(t)|)}{\delta^2} + \frac{|\dot{E}(t)|}{\delta^2} \right).$$

Since $E(t) = \mathrm{tr}(H(t)P(t))/\mathrm{tr}P(t)$, it follows from the differentiability of $P(t)$ and $H(t)$ that also $E(t)$ is continuously differentiable and therefore $\sup_{t\in J'}(|E(t)| + |\dot{E}(t)|) < \infty$. According to the assumptions on $H(t)$ we have $\sup_{t\in J'} \|\dot{H}(t)R(\mathrm{i}, t)\| = \sup_{t\in J'} \|(H(t) + \mathrm{i})\dot{R}(\mathrm{i}, t)\| < \infty$.

The crucial step in proving the adiabatic theorem without gap condition is to establish (6.13). However, this follows from Lemma 6.1. Since $P(t)$ has finite rank, $\lim_{\delta\to 0} \|Y_\delta(t)P(t)\| = 0$ follows if one can show $\lim_{\delta\to 0} \|Y_\delta(t)P(t)\psi\| = 0$ for all ψ. Let $\varphi := \dot{P}(t)P(t)\psi$, then, whenever $P(t)$ is spectral, Lemma 6.1 implies

$$\lim_{\delta\to 0} \|Y_\delta(t)P(t)\psi\|^2 = \lim_{\delta\to 0} \|\,\delta R(E(t) - \mathrm{i}\,\delta, t)\,(1 - P(t))\,\varphi\|^2 = 0\,,$$

where we used, as always, that $\varphi \in \mathrm{Ran}(1 - P(t))$ according to (6.11). Hence, $\lim_{\delta\to 0} \|Y_\delta(t)P(t)\psi\| = 0$ for almost all $t \in J'$. □

6.2 Space-adiabatic theory without gap condition

The time-adiabatic theorem without gap can be translated to perturbations of fibered Hamiltonians exactly as in the case of first order time-adiabatic theorem with gap, cf. Chapter 2. In this section we formulate a general space-adiabatic theorem without gap condition. However, compared to the pedagogical Section 2.2 we will drop several simplifying assumptions. As a consequence the general result can be directly applied to the massless Nelson model in Section 6.3.

For better readability we denote the configuration space of the slow degrees of freedom by $M = \mathbb{R}^d$. Let $H_0(x)$, $x \in M$, be a family of self-adjoint operators on some common dense domain $\mathcal{D} \subset \mathcal{H}_\mathrm{f}$, $\mathcal{H}_\mathrm{f}$ a separable Hilbert space. Let $\|\cdot\|_{H_0(x)}$ denote the graph norm of $H_0(x)$ on $\mathcal{D}$, i.e., for $\psi \in \mathcal{D}$, $\|\psi\|_{H_0(x)} = \|H_0(x)\psi\| + \|\psi\|$. We assume that all the $H_0(x)$-norms are equivalent in the sense that there is an $x_0 \in M$ and constants $C_1, C_2 < \infty$ such that $C_1\|\psi\|_{H_0(x_0)} \leq \|\psi\|_{H_0(x)} \leq C_2\|\psi\|_{H_0(x_0)}$. Then

$$H_0 = \int_M^\oplus \mathrm{d}x\, H_0(x)$$

with domain $D(H_0) = L^2(M) \otimes \mathcal{D}$ is self-adjoint, where here and in the following $\mathcal{D}$ resp. $D(H_0)$ are understood to be equipped with the $\|\cdot\|_{H_0(x_0)}$ resp. $\|\cdot\|_{H_0}$ norm. Let $m \geq 2$ and denote as before $R_0(\zeta, x) = (H_0(x) - \zeta)^{-1}$.

Condition $\mathbf{H}_0^m$. *Let $H_0(\cdot) \in C_\mathrm{b}^m(M, \mathcal{L}(\mathcal{D}, \mathcal{H}_\mathrm{f}))$ and for all $x \in M$ let $P_*(x)$ be an orthogonal projection such that $H_0(x)\,P_*(x) = E(x)\,P_*(x)$ with $P_*(\cdot) \in C_\mathrm{b}^{m+1}(M, \mathcal{L}(\mathcal{H}_\mathrm{f}))$ and $E(\cdot) \in C_\mathrm{b}^m(M, \mathbb{R})$.*

In addition one of the following assertions holds:

(i) *For $1 \leq j \leq n$*

$$\lim_{\delta \to 0} \operatorname*{ess\,sup}_{x \in M} \| \delta\, R_0(E(x) - \mathrm{i}\,\delta, x)\, (\partial_{x_j} P_*)(x) P_*(x)\|_{\mathcal{L}(\mathcal{H}_\mathrm{f})} = 0\,. \tag{6.14}$$

(ii) *There is a constant $\delta_0 > 0$ and a function $\eta : [0, \delta_0] \to [0, \delta_0]$ with $\eta(\delta) \geq \delta$ and a constant $C < \infty$ such that for $\delta \in (0, \delta_0]$ and $1 \leq j \leq n$*

$$\operatorname*{ess\,sup}_{x \in M} \| R_0(E(x) - \mathrm{i}\,\delta, x)\, (\partial_{x_j} P_*)(x) P_*(x)\|_{\mathcal{L}(\mathcal{H}_\mathrm{f})} \leq C\,\delta^{-1}\,\eta(\delta)\,. \tag{6.15}$$

(iii) *In addition to (6.15) for $1 \leq k, j \leq n$ also*

$$\operatorname*{ess\,sup}_{x \in M} \Big\| \partial_{x_k} \Big(R_0(E(x) - \mathrm{i}\,\delta, x)(\partial_{x_j} P_*)(x) P_*(x) \Big) \Big\|_{\mathcal{L}(\mathcal{H}_\mathrm{f})} \leq C\,\delta^{-1}\,\eta(\delta) \tag{6.16}$$

holds.

A few remarks concerning Condition $\mathbf{H}_0^m$ are in order:

– It is *not* assumed that $P_*(x)$ is the spectral projection of $H_0(x)$ corresponding to the eigenvalue $E(x)$. However, (6.14) holds pointwise in x whenever $P_*(x)$ is the spectral projection and has finite rank, cf. Proposition 6.4.
– Inequality (6.15) is always satisfied with $\eta(\delta) = 1$. For Condition $\mathbf{H}_0^m$ (ii) and (iii) to have nontrivial consequences on the rate of convergence in the adiabatic theorem, $\eta(\delta)$ must satisfy $\lim_{\delta\to 0}\eta(\delta) = 0$. These assumptions might look rather artificial at first sight, but turn out to be very natural in the proof and also in our application.
– The regularity of $P_*(x)$ has to be assumed, since it does not follow from the regularity of $H_0(x)$ without the gap condition, even if $P_*(x)$ is spectral. The regularity of $E(x)$ follows from the one of $H_0(x)$ and $P_*(x)$ whenever $P_*(x)$ has finite rank, as can be seen by writing $E(x) = \mathrm{tr}(H_0(x)P_*(x))/\mathrm{tr}P_*(x)$.

The "band subspace" $P_*\mathcal{H}$ defined through $P_* = \int_M^{\oplus} \mathrm{d}x\, P_*(x)$ is invariant under the dynamics generated by H_0, since $[H_0, P_*] = 0$ holds by construction. We will consider perturbations h^ε of H_0 satisfying

Condition $\mathbf{h}^m$. *For $\varepsilon \in (0,1]$ let h^ε be a self-adjoint operator with domain $D(h) \subset \mathcal{H}$ independent of ε such that $H_0 + h^\varepsilon$ is essentially self-adjoint on $D(h) \cap D(H_0)$. There exists an operator $(Dh)^\varepsilon \in \mathcal{L}_{\mathrm{sa}}(\mathcal{H})^{\oplus d}$ with $\sup_{\varepsilon\in(0,1]} \|\,|\,(Dh)^\varepsilon\,|\,\|_{\mathcal{L}(\mathcal{H})} < \infty$ satisfying:*

(i) *There is a constant $C < \infty$ such that for each $A \in C_{\mathrm{b}}^m(M, \mathcal{L}(\mathcal{H}_{\mathrm{f}}))$*

$$\|[h^\varepsilon, A] + \mathrm{i}\,\varepsilon\,\nabla_x A \cdot (Dh)^\varepsilon\|_{\mathcal{L}(\mathcal{H})} \leq C \sum_{j=2}^{m} \varepsilon^j \sup_{x\in M,\,|\alpha|=j} \|\partial_x^\alpha A(x)\|_{\mathcal{L}(\mathcal{H}_{\mathrm{f}})}\,.$$

(ii) *There is a constant $C < \infty$ such that*

$$\|\,|\,[(Dh)^\varepsilon, H_0]\,|\,\|_{\mathcal{L}(D(H_0),\mathcal{H})} + \|\,|\,[(Dh)^\varepsilon, h^\varepsilon]\,|\,\|_{\mathcal{L}(\mathcal{H})} \leq \varepsilon\, C\,.$$

By assumption, $H^\varepsilon = H_0 + h^\varepsilon$ is essentially self-adjoint on $D(h) \cap D(H_0)$ and we use its closure, again denoted by H^ε, to define for $t \in \mathbb{R}$

$$U^\varepsilon(t) = \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}\,.$$

Since, according to Assumption $\mathbf{h}^m$ (i), $[H^\varepsilon, P_*] = [h^\varepsilon, P_*] = \mathcal{O}(\varepsilon)$, the naive argument gives $[U^\varepsilon(t), P_*] = |t|\mathcal{O}(1)$. Indeed, our aim is again to cure the failure of the naive argument and to show that $P_*\mathcal{H}$ is invariant for $U^\varepsilon(t)$ in the limit $\varepsilon \to 0$. To this end we will, as in Chapter 2, compare $U^\varepsilon(t)$ with the unitary group generated by

$$H^\varepsilon_{\mathrm{diag}} \;=\; H_0 \;+\; P_*\, h^\varepsilon\, P_* \;+\; P_*^\perp\, h^\varepsilon\, P_*^\perp\,.$$

Also $H^\varepsilon_{\mathrm{diag}}$ is self-adjoint on $D(H^\varepsilon)$ since $P_*(\cdot) \in C_{\mathrm{b}}^m(M, \mathcal{L}(\mathcal{H}_{\mathrm{f}}))$ and thus $H^\varepsilon - H^\varepsilon_{\mathrm{diag}} = P_*^\perp[h^\varepsilon, P_*]P_* - P_*[h^\varepsilon, P_*]P_*^\perp$ is bounded according to $\mathbf{h}^m$ (i). Again we abbreviate for $t \in \mathbb{R}$

$$U^{\varepsilon}_{\mathrm{diag}}(t) = \mathrm{e}^{-\mathrm{i}H^{\varepsilon}_{\mathrm{diag}}t/\varepsilon}\,,$$

and we have by construction that

$$\big[P_*, U^{\varepsilon}_{\mathrm{diag}}(t)\big] = 0\,,$$

i.e. $P_*\mathcal{H}$ and $P_*^{\perp}\mathcal{H}$ are invariant subspaces for the dynamics generated by $H^{\varepsilon}_{\mathrm{diag}}$.

Theorem 6.3. *Assume* $\mathbf{H}_0^m$ *and* $\mathbf{h}^m$ *for some* $m \geq 2$. *Let* $\varepsilon \in (0, \delta_0]$, *then*

– $\mathbf{H}_0^m$ (i) *implies that for* $t \in \mathbb{R}$

$$\lim_{\varepsilon\to 0} \Big\| U^{\varepsilon}(t) - U^{\varepsilon}_{\mathrm{diag}}(t) \Big\|_{\mathcal{L}(\mathcal{H})} = 0\,, \tag{6.17}$$

– $\mathbf{H}_0^m$ (ii) *implies that for some constant* $C < \infty$ *and all* $t \in \mathbb{R}$

$$\Big\| U^{\varepsilon}(t) - U^{\varepsilon}_{\mathrm{diag}}(t) \Big\|_{\mathcal{L}(\mathcal{H})} \leq C\,\eta(\varepsilon^{\frac{1}{2}})\,(1+|t|)\,, \tag{6.18}$$

– $\mathbf{H}_0^m$ (iii) *implies that for some constant* $C < \infty$ *and all* $t \in \mathbb{R}$

$$\Big\| U^{\varepsilon}(t) - U^{\varepsilon}_{\mathrm{diag}}(t) \Big\|_{\mathcal{L}(\mathcal{H})} \leq C\,\eta(\varepsilon)\,(1+|t|)\,. \tag{6.19}$$

Note that in Theorem 6.3 the whole spectrum of possible rates of convergence between $o(1)$ and $\mathcal{O}(\varepsilon)$ as in the case with gap is covered. The estimates for the massless Nelson model as an application of Theorem 6.3 will show that, in principle, all rates can occur.

The following proposition shows that, assuming the first part of $\mathbf{H}_0^m$ but neither (i), (ii) or (iii), then Assumption $\mathbf{H}_0^m$ (i) always holds pointwise in x if $P_*(x)$ is the spectral projection and has finite rank. The proof is again an application of Lemma 6.1 analogous to the argument at the end of Section 6.1 in the time-adiabatic setting.

Proposition 6.4. *Assume* $\mathbf{H}_0^1$ *without (i), (ii) or (iii). If* $P_*(x)$ *is the spectral projection of* $H_0(x)$ *corresponding to the eigenvalue* $E(x)$ *and has finite rank, then*

$$\lim_{\delta\to 0} \| \,\delta\, R_0(E(x) - \mathrm{i}\delta, x)\,(\nabla_x P_*)(x) P_*(x)\|_{\mathcal{L}(\mathcal{H}_{\mathrm{f}})} = 0\,. \tag{6.20}$$

It is clear from (6.2) that additional information on the regularity of the spectral measure μ_φ provides some control on the rate of convergence in (6.20). E.g., if $\mu_\varphi(\mathrm{d}\lambda) = \rho_\varphi(\lambda)\mathrm{d}\lambda$ with $\rho_\varphi \in L^\infty(\mathbb{R}, \mathrm{d}\lambda)$, then

$$\int_{\mathbb{R}} \mu_\varphi(\mathrm{d}\lambda)\,\frac{\delta^2}{(\lambda - E(x))^2 + \delta^2} \;\leq\; \|\rho_\varphi\|_\infty \int_{\mathbb{R}} \mathrm{d}\lambda\,\frac{\delta^2}{(\lambda - E(x))^2 + \delta^2} = \mathcal{O}(\delta)$$

and hence (6.15) would hold pointwise in x with $\eta(\delta) = \delta^{1/2}$. In a sense, the rate $\mathcal{O}(\varepsilon\sqrt{\ln(1/\varepsilon)})$ for the massless Nelson model (6.57) is a consequence of the relevant spectral measure having a density $\rho(\lambda) \sim \lambda - E(x)$.

Remark 6.5. We emphasize that (6.20) for all $x \in M$ does *not* imply $\mathbf{H}_0^m$ (i), even in the case of compact M. This is because for pointwise convergence to imply uniform convergence one would need uniform equicontinuity of a sequence of functions. However, in the time-adiabatic setting it was sufficient to have (6.20) for almost all $t \in J'$, because of the integration over time in (6.10).

The fact that the uniform condition appears in the space-adiabatic theorem can be understood as follows. In the time-adiabatic setting all states move at a constant speed through points where the rate of convergence in (6.20) is very slow or where (6.20) fails completely, as e.g. at crossings. Thus, if they form a null-set, they can be ignored. On the other hand, in the space-adiabatic case some states may dwell near such bad points for long times and therefore the adiabatic decoupling can no longer hold uniform in all initial states. ♢

Proof (of Theorem 6.3). We start with the standard argument and find that on $D(H^\varepsilon)$

$$\begin{aligned} U^\varepsilon(t) - U^\varepsilon_{\mathrm{diag}}(t) &= -\,U^\varepsilon(t) \int_0^t \mathrm{d}t' \, \frac{\mathrm{d}}{\mathrm{d}t'} \left(U^\varepsilon(-t')\, U^\varepsilon_{\mathrm{diag}}(t') \right) \qquad (6.21) \\ &= -\,\frac{\mathrm{i}}{\varepsilon}\, U^\varepsilon(t) \int_0^t \mathrm{d}t' \, U^\varepsilon(-t') \left(H^\varepsilon \,-\, H^\varepsilon_{\mathrm{diag}} \right) U^\varepsilon_{\mathrm{diag}}(t') \,, \end{aligned}$$

where

$$H^\varepsilon \,-\, H^\varepsilon_{\mathrm{diag}} = P_*^\perp \, h^\varepsilon \, P_* \,+\, P_* \, h^\varepsilon \, P_*^\perp = P_*^\perp \left[h^\varepsilon, P_* \right] P_* \,+\, \text{adj.}\,. \qquad (6.22)$$

Inserting $\mathbf{h}^m$ (i) into (6.22) and the result back into (6.21) one obtains

$$\begin{aligned} &\left\| U^\varepsilon(t) - U^\varepsilon_{\mathrm{diag}}(t) \right\|_{\mathcal{L}(\mathcal{H})} = \qquad (6.23) \\ &= \left\| \int_0^t \mathrm{d}t' \, U^\varepsilon(-t') \, \left(P_*^\perp \, (\nabla_x P_*) \, P_* \cdot (Dh)^\varepsilon \, P_* \,+\, \text{adj.} \right) U^\varepsilon_{\mathrm{diag}}(t') \right\|_{\mathcal{L}(\mathcal{H})} \\ &\qquad + \mathcal{O}(\varepsilon)|t| \,. \end{aligned}$$

In (6.23) we used again

$$(\nabla_x P_*)(x) = P_*^\perp(x)(\nabla_x P_*)(x) P_*(x) + \text{ adj.}\,. \qquad (6.24)$$

In order to control the remaining term on the right hand side of (6.23) we proceed as in the time-adiabatic setting. In Section 2.2 we defined the operator $F(x)$, cf. (2.23), where

$$F(x) = R_0(E(x), x) \, (\nabla_x P_*)(x) \, P_*(x) \qquad (6.25)$$

in the case of an energy band. $F(x)$ is well defined and bounded if the eigenvalue $E(x)$ is separated from the rest of the spectrum of $H_0(x)$ by a gap and if $P_*(x)$ is spectral.

Recall that definition (6.25) was made to give $[H_0, F] = P_*^\perp \big(\nabla_x P_*\big) P_*$. However, in absence of a gap (6.25) is not well defined as an operator on $\mathcal{H}_\mathrm{f}$ and, as in Section 6.1, we shift the resolvent into the complex plane and define

$$F_\delta(x) = R_0(E(x) - \mathrm{i}\delta, x)\, P_*^\perp(x)\, (\nabla_x P_*)(x)\, P_*(x)\,.$$

One now obtains

$$\big[\, H_0(x)\,,\, F_\delta(x)\,\big] = P_*^\perp(x)\, \big(\nabla_x P_*\big)(x)\, P_*(x) + Y_\delta(x) \tag{6.26}$$

with

$$Y_\delta(x) = -\,\mathrm{i}\,\delta R_0(E(x) - \mathrm{i}\delta, x)\, (\nabla_x P_*)(x)\, P_*(x)\,. \tag{6.27}$$

Conditions $\mathbf{H}_0^m$ (i), (ii) and (iii) each imply that $\lim_{\delta\to 0} \|Y_\delta\|_{\mathcal{L}(\mathcal{H})} = 0$. To see this recall that for $A(\cdot) \in L^\infty(M, \mathcal{L}(\mathcal{H}_\mathrm{f}))$ one has

$$\|A\|_{\mathcal{L}(\mathcal{H})} = \operatorname*{ess\,sup}_{x\in M} \|A(x)\|_{\mathcal{L}(\mathcal{H}_\mathrm{f})}\,.$$

Note that for better readability we omit the Euclidean norm $|\ldots|$ in the notation and understand that $\|A\|$ always includes also the Euclidean norm if A is an operator with d components. Thus with (6.27) we can make the remainder in (6.26) arbitrarily small by choosing δ small enough. However, for the time being we let $\delta > 0$ but carefully keep track of the dependence of all errors on δ.

By assumption $H_0(\cdot) \in C_\mathrm{b}^m(M, \mathcal{L}(\mathcal{D}, \mathcal{H}_\mathrm{f}))$ and $P_*(\cdot) \in C_\mathrm{b}^{m+1}(M, \mathcal{L}(\mathcal{H}_\mathrm{f}))$, which implies $F_\delta(\cdot) \in C_\mathrm{b}^m(M, \mathcal{L}(\mathcal{H}_\mathrm{f})^{\oplus d})$ and hence, according to $\mathbf{h}^m$ (i),

$$\Big\|\, \big[h^\varepsilon, F_\delta\,\big]\,\Big\|_{\mathcal{L}(\mathcal{H})} \;\leq\; C \sum_{j=1}^{m} \varepsilon^j \sup_{|\alpha|=j} \|\,\partial_x^\alpha F_\delta\,\|_{\mathcal{L}(\mathcal{H})} =: f_1(\varepsilon, \delta)\,. \tag{6.28}$$

Combining (6.26) and (6.28) we obtain

$$\big[\, H^\varepsilon, F_\delta\,\big] \;=\; P_*^\perp \big(\nabla_x P_*\big)\, P_* \;+ \mathcal{O}(\|Y_\delta\|, f_1(\varepsilon, \delta))\,, \tag{6.29}$$

where in (6.29) and in the following $\mathcal{O}(a, b, c, \ldots)$ stands for a sum of operators whose norm in $\mathcal{L}(\mathcal{H})$ is bounded by a constant times $a + b + c + \ldots$. Defining

$$B_\delta = F_\delta \cdot (Dh)^\varepsilon\, P_* - \mathrm{adj.}\,,$$

one finds with $\mathbf{h}^m$ (ii) and $f_2(\delta) = \|F_\delta\|_{\mathcal{L}(\mathcal{H}, D(H_0))}$ that

$$\begin{aligned}\big[H^\varepsilon, B_\delta\,\big] &= \big[H^\varepsilon, F_\delta\,\big] \cdot (Dh)^\varepsilon\, P_* \;+ F_\delta \cdot \big[H^\varepsilon, (Dh)^\varepsilon\big]\, P_* \\ &\qquad + F_\delta \cdot (Dh)^\varepsilon \,\big[H^\varepsilon,\, P_*\big] + \mathrm{adj.} \\ &= P_*^\perp \big(\nabla_x P_*\big)\, P_* \cdot (Dh)^\varepsilon \;+ \mathrm{adj.} \;+\; \mathcal{O}(\varepsilon, \|Y_\delta\|, f_1(\varepsilon, \delta), \varepsilon f_2(\delta))\,.\end{aligned} \tag{6.30}$$

Now the integrand in (6.23) can be written as the time-derivative of

$$A_\delta(t) = -\,\mathrm{i}\,\varepsilon\, U^\varepsilon(-t)\, B_\delta\, U^\varepsilon(t)\,,$$

plus a remainder:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}A_\delta(t) &= U^\varepsilon(-t)\,[H^\varepsilon, B_\delta]\,U^\varepsilon(t)\\ &= U^\varepsilon(-t)\,\left(P_*^\perp\left(\nabla_x P_*\right)P_*\cdot(Dh)^\varepsilon\,P_* + \text{adj.}\right)U^\varepsilon(t)\\ &\quad + \mathcal{O}(\varepsilon, \|Y_\delta\|, f_1(\varepsilon,\delta), \varepsilon f_2(\delta))\,. \end{aligned} \tag{6.31}$$

Inserting (6.31) into (6.23) enables us to do integration by parts,

$$\begin{aligned}&\left\|U^\varepsilon(t) - U^\varepsilon_{\mathrm{diag}}(t)\right\|_{\mathcal{L}(\mathcal{H})} \le\\ &\quad\le \left\| \int_0^t \mathrm{d}t'\, \left(\frac{\mathrm{d}}{\mathrm{d}t'}A_\delta(t')\right) U^\varepsilon(-t')\, U^\varepsilon_{\mathrm{diag}}(t') \right\|_{\mathcal{L}(\mathcal{H})}\\ &\qquad\qquad + |t|\,\mathcal{O}\Big(\varepsilon, \|Y_\delta\|, f_1(\varepsilon,\delta), \varepsilon f_2(\delta)\Big)\\ &\quad\le \|A_\delta(t)\|_{\mathcal{L}(\mathcal{H})} + \|A_\delta(0)\|_{\mathcal{L}(\mathcal{H})}\\ &\qquad + \left\| \int_0^t \mathrm{d}t'\, A_\delta(t') \left(\frac{\mathrm{d}}{\mathrm{d}t'}U^\varepsilon(-t')\, U^\varepsilon_{\mathrm{diag}}(t')\right)\right\|_{\mathcal{L}(\mathcal{H})}\\ &\qquad + |t|\,\mathcal{O}\Big(\varepsilon, \|Y_\delta\|, f_1(\varepsilon,\delta), \varepsilon f_2(\delta)\Big)\\ &\quad\le C\,\varepsilon\,(2+|t|)\,\|F_\delta\|_{\mathcal{L}(\mathcal{H})} + |t|\,\mathcal{O}\Big(\varepsilon, \|Y_\delta\|, f_1(\varepsilon,\delta), \varepsilon f_2(\delta)\Big)\,. \end{aligned} \tag{6.32}$$

For the last inequality in (6.32) we used that $\|A_\delta(t)\|_{\mathcal{L}(\mathcal{H})} \le C\,\varepsilon \|F_\delta\|_{\mathcal{L}(\mathcal{H})}$ uniformly for $t \in \mathbb{R}$ and that

$$\frac{\mathrm{d}}{\mathrm{d}t}\, U^\varepsilon(t)\, U^\varepsilon_{\mathrm{diag}}(t) = -\frac{\mathrm{i}}{\varepsilon}\, U^\varepsilon(t)\left(H^\varepsilon(t) \,-\, H^\varepsilon_{\mathrm{diag}}(t)\right) U^\varepsilon_{\mathrm{diag}}(t)$$

is bounded uniformly, according to (6.22) and $\mathbf{h}^m$ (i).

Writing out the various terms in (6.32) explicitly, we conclude that there is a constant $C < \infty$ such that

$$\begin{aligned}\left\|U^\varepsilon(t) - U^\varepsilon_{\mathrm{diag}}(t)\right\|_{\mathcal{L}(\mathcal{H})} &\le C\,\varepsilon\,\|F_\delta\|_{\mathcal{L}(\mathcal{H})} + C\,|t|\,\Big(\varepsilon + \|Y_\delta\|_{\mathcal{L}(\mathcal{H})}\\ &\quad + \varepsilon\,\|F_\delta\|_{\mathcal{L}(\mathcal{H},D(H_0))} + \varepsilon\,\|F_\delta\|_{\mathcal{L}(\mathcal{H})} + \sum_{j=1}^m \varepsilon^j \sup_{|\alpha|=j} \|\partial_x^\alpha F_\delta\|_{\mathcal{L}(\mathcal{H})}\Big)\,. \end{aligned} \tag{6.33}$$

Hence we are left to establish bounds on F_δ, on its derivatives and on Y_δ in terms of δ, which is the content of the following Lemma.

Lemma 6.6. *Assume $\mathbf{H}_0^m$, then $F_\delta(\cdot) \in C^m_{\mathrm{b}}(M, \mathcal{L}(\mathcal{H}_{\mathrm{f}})^{\oplus d})$ and there is a constant $C < \infty$ such that for $\delta \in (0, \delta_0]$*

$$\|F_\delta\|_{\mathcal{L}(\mathcal{H},D(H_0))} \le \frac{C}{\delta}\,\eta(\delta)\,, \tag{6.34}$$

$$\sup_{|\alpha|=j} \| \partial_x^\alpha F_\delta \|_{\mathcal{L}(\mathcal{H})} \leq \frac{C}{\delta^{j+1}} \eta(\delta) \quad \textit{for } 1 \leq j \leq m\,. \tag{6.35}$$

In case $\mathbf{H}_0^m$ (i) *holds, we have (6.34) and (6.35) with* $\eta(\delta) = 1$. *Furthermore, if* $\mathbf{H}_0^m$ (i) *holds, then* $\lim_{\delta\to 0} \|Y_\delta\|_{\mathcal{L}(\mathcal{H})} = 0$ *and if* $\mathbf{H}_0^m$ (ii) *or* (iii) *holds, then* $\|Y_\delta\|_{\mathcal{L}(\mathcal{H})} \leq C\,\eta(\delta)$.

If $\mathbf{H}_0^m$ *(iii) holds, then (6.35) can be improved to*

$$\sup_{|\alpha|=j} \| \partial_x^\alpha F_\delta \|_{\mathcal{L}(\mathcal{H})} \leq \frac{C}{\delta^{j}} \eta(\delta) \quad \textit{for } 1 \leq j \leq m\,. \tag{6.36}$$

Before we turn to the proof of Lemma 6.6 we finish the proof of Theorem 6.3. Assuming $\mathbf{H}_0^m$ (i), (6.17) follows by inserting the bounds from Lemma 6.6 into (6.33) and choosing $\delta = \delta(\varepsilon)$ such that $\lim_{\varepsilon\to 0} \delta(\varepsilon) = 0$ and $\lim_{\varepsilon\to 0} \varepsilon/\delta(\varepsilon)^2 = 0$.

If $\mathbf{H}_0^m$ (ii) holds, then the bounds (6.34) and (6.35) inserted into (6.33) yield

$$\big\|U^\varepsilon(t) - U^\varepsilon_{\mathrm{diag}}(t)\big\|_{\mathcal{L}(\mathcal{H})} \leq C\,\varepsilon\,\frac{\eta(\delta)}{\delta} + C\,\Big(\varepsilon + \eta(\delta) + \varepsilon\,\frac{\eta(\delta)}{\delta} + \sum_{j=1}^{m} \varepsilon^j\,\frac{\eta(\delta)}{\delta^{j+1}}\Big)|t|\,. \tag{6.37}$$

In (6.37) the optimal choice is $\delta(\varepsilon) = \varepsilon^{\frac{1}{2}}$, which gives (6.18). Finally, the bounds (6.34) and (6.36) inserted into (6.33) yield

$$\big\|U^\varepsilon(t) - U^\varepsilon_{\mathrm{diag}}(t)\big\|_{\mathcal{L}(\mathcal{H})} \leq C\,\varepsilon\,\frac{\eta(\delta)}{\delta} + C\,\Big(\varepsilon + \eta(\delta) + \varepsilon\,\frac{\eta(\delta)}{\delta} + \sum_{j=1}^{m} \varepsilon^j\,\frac{\eta(\delta)}{\delta^{j}}\Big)|t|\,,$$

where the optimal choice $\delta(\varepsilon) = \varepsilon$ gives (6.19). □

Proof (of Lemma 6.6). We abbreviate $R_0(E(x) - \mathrm{i}\delta, x)$ as $R(\delta, x)$ in this proof and note that $R(\delta,\cdot) \in C^m_{\mathrm{b}}(M, \mathcal{L}(\mathcal{H}_{\mathrm{f}}))$ and thus $F_\delta(\cdot) \in C^m_{\mathrm{b}}(M, \mathcal{L}(\mathcal{H}_{\mathrm{f}})^{\oplus d})$ follow from $H_0(\cdot) \in C^m_{\mathrm{b}}(M, \mathcal{L}(\mathcal{D}, \mathcal{H}_{\mathrm{f}}))$ together with $P_*(\cdot) \in C^{m+1}_{\mathrm{b}}(M, \mathcal{L}(\mathcal{H}_{\mathrm{f}}))$.

We start with the case $\mathbf{H}_0^m$ (ii), where (i) is included by making the obvious changes for $\eta(\delta) = 1$. Assumption $\mathbf{H}_0^m$ (ii) immediately yields

$$\|F_\delta\|_{\mathcal{L}(\mathcal{H})} \leq \frac{C}{\delta}\,\eta(\delta) \tag{6.38}$$

and the bound on Y_δ. (6.34) follows from $H_0(x)R(\delta,x) = \mathbf{1} + (E(x) - \mathrm{i}\delta)R(\delta,x)$ and (6.38) together with the assumption that $E(x)$ is uniformly bounded.

For (6.35) we start by observing that

$$\begin{aligned} \nabla_x F_\delta(x) &= R(\delta,x)\,\nabla_x\Big((\nabla_x P_*)(x)P_*(x)\Big) \\ &\quad + \Big(\nabla_x R(\delta,x)\Big)(\nabla_x P_*)(x)P_*(x) \\ &= R(\delta,x)\nabla_x\Big((\nabla_x P_*)(x)P_*(x)\Big) \\ &\quad - R(\delta,x)(\nabla_x H_0(x) - \nabla_x E(x))F_\delta(x). \end{aligned} \tag{6.39}$$

Using (6.38) and the fact that $|\nabla_x E(x)|$ is uniformly bounded by assumption, we infer from (6.39) that

$$\| \, |\nabla_x F_\delta| \, \|_{\mathcal{L}(\mathcal{H})} = \sup_{x \in M} \| \, |\nabla_x F_\delta(x)| \, \|_{\mathcal{L}(\mathcal{H}_{\rm f})} \leq C(\delta^{-1} + \delta^{-2}\eta(\delta)) \, .$$

Hence (6.35) follows for $j = 1$, since $\delta \leq \eta(\delta)$ by assumption.

By differentiating (6.39) again, we find, using a reduced notation with obvious meaning, that

$$\begin{aligned} \nabla^{(2)} F_\delta = -2R_\delta (\nabla H_0 - \nabla E) \, \nabla F_\delta + R_\delta \, \nabla^{(2)} \Big((\nabla P_*) P_* \Big) \\ - R_\delta (\nabla^{(2)} H_0 - \nabla^{(2)} E) \, F_\delta \, . \end{aligned} \tag{6.40}$$

Hence $\|\nabla^{(2)} F_\delta\|_{\mathcal{L}(\mathcal{H})} \leq C(\delta^{-3}\eta(\delta) + \delta^{-1} + \delta^{-2}\eta(\delta))$ which proves (6.35) for $j = 2$. By repeated differentiation one finds inductively (6.35) for $j \leq m$.

To show (6.36) assuming $\mathbf{H}_0^m$ (iii), note that (6.36) holds by assumption for $j = 1$ and inserted into (6.40) it gives $\|\nabla^{(2)} F_\delta\|_{\mathcal{L}(\mathcal{H})} \leq C(\delta^{-2}\eta(\delta) + \delta^{-1} + \delta^{-2}\eta(\delta))$. Analogously the estimates for all larger $j \leq m$ are improved by a factor of δ. □

6.3 Effective N-body dynamics in the massless Nelson model

The physical picture underlying nonrelativistic quantum electrodynamics is that of charged particles which interact through the exchange of photons and dissipate energy through emission of photons. In situations where the velocities of the particles are small compared to the propagation speed of the photons the interaction is given through effective, instantaneous pair potentials. If, in addition, also accelerations are small, then dissipation through radiation can be neglected in good approximation. Instead of full nonrelativistic QED we consider the massless Nelson model. This model describes N *spinless* particles coupled to a *scalar* Bose field of zero mass.

The content of this section is a mathematical derivation of the time-dependent Schrödinger equation for N particles with Coulombic pair potentials from the massless Nelson model with ultraviolet cutoffs. The key ingredient is the space-adiabatic theorem without gap condition of Section 6.2.

6.3.1 Formulation of the problem

Before we turn to a more careful discussion of the type of scaling we shall consider, notice that the coupling of N *noninteracting* particles to the radiation field has *three* effects.

– The effective mass, or more precisely, the effective dispersion relation of the particles is modified. The term "effective" refers to the reaction of the particles to weak external forces. The physical picture is that each particle now carries a cloud of photons with it, which makes it heavier.
– The particles feel an interaction mediated through the field. If the propagation speed of the particles is small compared to the one of the photons, then retardation effects should be negligible and the interaction between the particles can be described in good approximation by instantaneous pair potentials.
– Energy is dissipated through photons moving freely to infinity. The motion of the particles is, in general, no longer of Hamiltonian type. The rate of energy emitted as photons is proportional to the acceleration of a particle squared.

The scaling to be studied is most conveniently explained on the classical level. The classical equations of motion for N particles with positions q_j, masses m_j and rigid "charge" distributions ρ_j coupled to the scalar field $\phi(x,t)$ with propagation speed c are

$$\frac{1}{c^2}\,\ddot{\phi}(x,t) = \Delta_x\phi(x,t) - \sum_{j=1}^{N} \rho_j(x-q_j(t)) \tag{6.41}$$

$$m_j\,\ddot{q}_j(t) = -\int_{\mathbb{R}^3} \mathrm{d}x\,(\nabla_x\phi)(x,t)\,\rho_j(x-q_j(t))\,, \quad 1\le j\le N\,. \tag{6.42}$$

One can think of $\rho_j(x) = e_j\,\varphi(x)$ as a smeared out point charge e_j with a form factor $\varphi \ge 0$ satisfying $\int_{\mathbb{R}^3}\mathrm{d}x\,\varphi(x) = 1$. Taking the limit $c\to\infty$ in (6.41) yields the Poisson equation for the field and thus, after elimination of the field, (6.42) describes N particles interacting through smeared Coulomb potentials. Mass renormalization for the particles in not visible at leading order.

Instead of taking $c\to\infty$ one can as well explore for which scaling of the particle properties one obtains analogous effective equations. Since retardation effects should be negligible, the initial velocities of the particles are now assumed to be $\mathcal{O}(\varepsilon)$ compared to the fixed propagation speed $c = 1$ of the field, $\varepsilon \ll 1$. In order to see motion of the particles over finite distances, we have to follow this dynamics at least over times of order $\mathcal{O}(\varepsilon^{-1})$. To make sure that the velocities are still of order $\mathcal{O}(\varepsilon)$ after times of order $\mathcal{O}(\varepsilon^{-1})$, the accelerations must be at most of order $\mathcal{O}(\varepsilon^2)$. The last constraint also guarantees that the energy dissipated over times of order $\mathcal{O}(\varepsilon^{-1})$ is at most of order $\mathcal{O}(\varepsilon^3)$.

The natural procedure would now be to consider such initial data, for which the velocities stay of order $\mathcal{O}(\varepsilon)$ over sufficiently long times. The problem simplifies if we assume, as we shall do in this work, that the mass of a particle is of order $\mathcal{O}(\varepsilon^{-2})$. As a consequence accelerations are and stay of order $\mathcal{O}(\varepsilon^2)$ *uniformly for all initial conditions*. In this scaling limit mass

renormalization is *not* visible at leading order. Indeed, if we substitute $t' = \varepsilon t$ and $m'_j = \varepsilon^2 m_j$ in (6.41) and (6.42), we find that the limit $\varepsilon \to 0$ is equivalent to the limit $c \to \infty$.

After quantization, however, the two limiting procedures are no longer equivalent. The limit $c \to \infty$ for the Nelson model was analyzed by Davies [Da] and later also by Hiroshima [Hi], who removed the ultraviolet cutoff. A comparison of their results with ours can be found at the end of this introduction. We will adopt the point of view that it is more natural to explore the regime of particle properties which gives rise to effective equations than to take the limit $c \to \infty$.

The deeper reason for our choice is that the more natural procedure of restricting to appropriate initial conditions gives rise to a similar mathematical structure. If the bare mass of the particles of order $\mathcal{O}(1)$, then the proper scaling which yields effective equations with renormalized masses was introduced and analyzed for the classical Abraham model by Kunze and Spohn, see [KuSp, Sp_2] and references therein. Denoting again the ratio of the velocities of the particles and the field as ε, they consider charges initially separated by distances of order $\mathcal{O}(\varepsilon^{-2})$ in units of their diameter. Hence the forces are $\mathcal{O}(\varepsilon^4)$ initially. For times up to order $\mathcal{O}(\varepsilon^{-3})$ and for appropriate initial conditions – excluding head on collisions – the separation of the particles remains of order $\mathcal{O}(\varepsilon^{-2})$ and thus the velocities remain of order $\mathcal{O}(\varepsilon)$. In particular, the rescaled macroscopic position $q'(t') = \varepsilon^{-2}\, q(t'/\varepsilon^3)$ satisfies $(\mathrm{d}/\mathrm{d}t')^2\, q'(t') = \mathcal{O}(\varepsilon^4)$, which matches the order of the forces. As a consequence one obtains a sensible limiting dynamics for the macroscopic variables.

One would expect that the same scaling limit applied to the quantum mechanical model yields in a similar fashion effective dynamics with renormalized dispersion. However, inserting this scaling into the massless Nelson model, one faces mathematical problems beyond those in the simpler $m = \mathcal{O}(\varepsilon^{-2})$ scaling. Without going into details we remark that the main problem is that for massless bosons the Hamiltonian at fixed total momentum does not have a ground state in Fock space, cf. [Fr_1, Ch]. (As a consequence it is not even clear how to translate the result in [TeSp] for a *single quantum* particle coupled to a *massive* quantized scalar field and subject to weak external forces to the massless case.) Nevertheless, the simpler scaling with $m = \mathcal{O}(\varepsilon^{-2})$ provides at least a first step in the right direction, since the mechanism of adiabatic decoupling without gap will certainly play a crucial role also in a more refined analysis.

In the remainder of this introductory section we briefly present the massless Nelson model, explain our main result and compare it to Davies' "weak coupling limit" [Da].

Up to a modified dispersion for the particles, the following model is obtained through canonical quantization of the classical system (6.41) and (6.42). The state space for N spinless particles is $L^2(\mathbb{R}^{3N})$ and as Hamil-

tonian we take

$$H_{\mathrm{p}} = \sum_{j=1}^{N} \sqrt{-c_{\max}^2 \Delta_{x_j} + c_{\max}^4 m^2}\,, \tag{6.43}$$

where $c_{\max}$ is the maximally attainable speed of the particles and m their mass, $\hbar = 1$. As explained before, we consider the scaling limit

$$\varepsilon \ll 1 \quad \text{with} \quad c_{\max} = \mathcal{O}(\varepsilon) \quad \text{and} \quad m = \mathcal{O}(\varepsilon^{-2})\,. \tag{6.44}$$

It might seem somewhat artificial to have a relativistic dispersion relation for the particles which does not contain the speed of light, but some other maximal speed $c_{\max}$. This is done only for the sake of simple presentation. We could as well consider the quadratic dispersion $H_{\mathrm{p}} = -\sum_{j=1}^{N} \frac{1}{2m} \Delta_{x_j}$ for the particles. However, there would be no maximal speed and we would be forced to either introduce a cutoff for large momenta or to change the topology in (6.57). While both strategies are technically straightforward by using exactly the same methods as in Section 2.3 in the context of Born-Oppenheimer approximation, they would obscure the simple structure of our result.

We insert the scaling (6.44) into (6.43) and change units such that the particle Hamiltonian is now given through

$$H_{\mathrm{p}}^{\varepsilon} = \sum_{j=1}^{N} \sqrt{-\varepsilon^2 \Delta_{x_j} + 1}\,. \tag{6.45}$$

The particles are coupled to a scalar field whose state is an element of the bosonic Fock space over $L^2(\mathbb{R}^3)$ given as

$$\mathcal{F} = \oplus_{m=0}^{\infty} \otimes_{(\mathrm{s})}^{m} L^2(\mathbb{R}^3)\,, \tag{6.46}$$

where $\otimes_{(\mathrm{s})}^{m}$ is the m-times symmetric tensor product and $\otimes_{(\mathrm{s})}^{0} L^2(\mathbb{R}^3) := \mathbb{C}$. The Hamiltonian for the free bosonic field is

$$H_{\mathrm{f}} = \mathrm{d}\Gamma(|k|)\,, \tag{6.47}$$

where k is the boson momentum. In our units the propagation speed of the bosons is equal to one. The reader who is not familiar with the notation is asked to consult the beginning of Section 6.3.2, where the model is introduced in full detail.

In the standard Nelson model the coupling between the j^{th} particle and the field is given through

$$H_{\mathrm{I},j} = \int_{\mathbb{R}^3} \mathrm{d}y\, \phi(y)\, \rho_j(y - x_j)\,, \tag{6.48}$$

where ϕ is the field operator in position representation and x_j the position of the j^{th} particle. The charge density $\rho_j \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ of the j^{th} particle

is assumed to be spherically symmetric and its Fourier transform is denoted by $\hat{\rho}_j$. For the moment we also assume an infrared condition, namely that

$$\sum_{j=1}^{N} \frac{\hat{\rho}_j(k)}{|k|^{3/2}} \in L^2(\mathbb{R}^3)\,. \tag{6.49}$$

Condition (6.49) constrains the total charge of the system but *not* that of an individual particle to zero. The state of the combined particles + field system is an element of

$$\mathcal{H} = L^2(\mathbb{R}^{3N}) \otimes \mathcal{F}$$

and its time evolution is generated by the Hamiltonian

$$H^\varepsilon = H_{\mathrm{p}}^\varepsilon \otimes \mathbf{1} + \mathbf{1} \otimes \mathrm{d}\Gamma(|k|) + \sum_{j=1}^{N} H_{\mathrm{I},j}\,. \tag{6.50}$$

Note that H contains no terms which directly couple different particles. All interactions between the particles must be mediated through the boson field.

Our goal is the construction of approximate solutions of the time dependent Schrödinger equation

$$\mathrm{i}\,\varepsilon \frac{\mathrm{d}}{\mathrm{d}t}\,\Psi(t) = H^\varepsilon \Psi(t)\,, \quad \Psi(0) = \Psi_0 \in \mathcal{H} \tag{6.51}$$

from solutions of an effective Schrödinger equation

$$\mathrm{i}\,\varepsilon \frac{\mathrm{d}}{\mathrm{d}t}\,\psi(t) = H_{\mathrm{eff}}^\varepsilon \psi(t)\,, \quad \psi(0) = \psi_0 \in L^2(\mathbb{R}^{3N}) \tag{6.52}$$

for the particles only. Notice the factor ε in front of the time derivative in (6.51) and (6.52), which means that we switched to a time scale of order ε^{-1} in microscopic units. As explained before, this is necessary in order to see nontrivial dynamics of the particles, since their speed is $\mathcal{O}(\varepsilon)$.

We remark that the scaling (6.44) coincides with the one in time-dependent Born-Oppenheimer approximation of Section 2.3, where $m = \mathcal{O}(\varepsilon^{-2})$ is the mass of the nuclei and where, at fixed kinetic energy, the velocities of the nuclei are also of order $\mathcal{O}(\varepsilon)$. The Hamiltonian (6.50) has the same structure as the molecular Hamiltonian and the role of the electrons in the Born-Oppenheimer approximation is now played by the bosons.

The key observation for the following is that the interaction Hamiltonian depends only on the configuration x of the particles and that the operator

$$H_0(x) = \mathrm{d}\Gamma(|k|) + \sum_{j=1}^{N} H_{\mathrm{I},j}(x)\,,$$

which acts on $\mathcal{F}$ for fixed $x \in \mathbb{R}^{3N}$, has a unique ground state $\Omega(x)$ with ground state energy

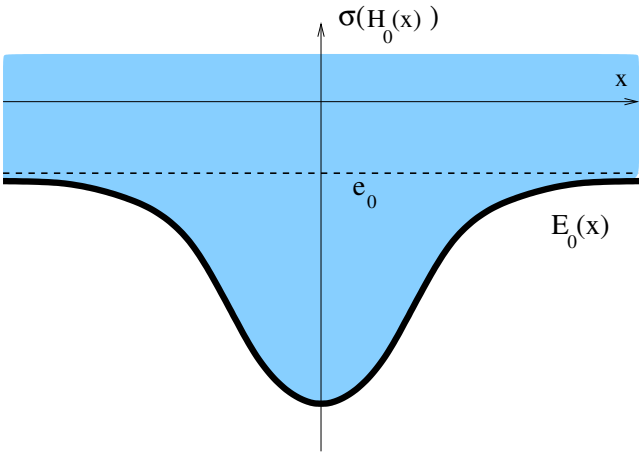

Fig. 6.1. The spectrum of $H_0(x)$ for $N = 2$. The thick line indicates the eigenvalue $E_0(x)$ sitting at the bottom of continuous spectrum.

$$E_0(x) = \sum_{j=2}^{N} \sum_{i=1}^{j-1} V_{ij}(x_i - x_j) + e_0 \,, \tag{6.53}$$

where

$$V_{ij}(z) = -\int_{\mathbb{R}^3 \times \mathbb{R}^3} \mathrm{d}v \, \mathrm{d}w \, \frac{\rho_i(v-z)\rho_j(w)}{4\pi|v-w|} \tag{6.54}$$

and

$$e_0 = -\frac{1}{2} \sum_{j=1}^{N} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \mathrm{d}v \, \mathrm{d}w \, \frac{\rho_j(v)\rho_j(w)}{4\pi|v-w|} \,. \tag{6.55}$$

$V_{ij}(z)$ is the electrostatic interaction energy of the charge distributions ρ_i and ρ_j at distance z, however, with the "wrong" sign. However, it is a peculiarity of the electromagnetic field that the interaction between charges with equal sign is repulsive. e_0 is the sum of all self energies. The remainder of the spectrum is purely absolutely continuous and the ground state energy is *not* isolated, cf. Figure 6.1.

Let $P_*(x) = |\Omega(x)\rangle\langle\Omega(x)|$, then the states in

$$P_*\mathcal{H} = \left\{ \int_{\mathbb{R}^{3N}}^{\oplus} \mathrm{d}x \, \psi(x)\Omega(x) : \ \psi \in L^2(\mathbb{R}^{3N}) \right\} \subset \mathcal{H} \tag{6.56}$$

correspond to wave packets without free bosons. These states are sections of ground states, not sections of vacua, and as such contain what is called "virtual" bosons in physics. States in $\mathrm{Ran}P_*$ could be called dressed many-particle states, since the particles carry a cloud of virtual bosons. If the particles are moving at small speeds and if the accelerations are also small, one expects

that no free bosons are created, i.e. that $P_*\mathcal{H}$ is approximately invariant under the dynamics generated by H^ε. Moreover the wave function $\psi(x)$ of the particles should approximately be governed by the effective Schrödinger equation (6.52) with

$$H^\varepsilon_{\text{eff}} = \sum_{j=1}^{N} \sqrt{-\varepsilon^2\Delta_{x_j} + 1} + \sum_{j=2}^{N}\sum_{i=1}^{j-1} V_{ij}(x_i - x_j)\,.$$

Our main result, Theorem 6.10, states that for $\Psi_0 = \int^\oplus \mathrm{d}x\, \psi_0(x)\Omega(x) \in P_*\mathcal{H}$ we have

$$\begin{aligned}\Big\| \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}\Psi_0 - \int_{\mathbb{R}^{3N}}^{\oplus} \mathrm{d}x \left(\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\text{eff}} t/\varepsilon}\,\psi_0\right)(x)\, \mathrm{e}^{-\mathrm{i}e_0 t/\varepsilon}\,\Omega(x)\Big\| \\ = \mathcal{O}(\varepsilon\sqrt{\ln(1/\varepsilon)})\,(1+|t|)\,\|\Psi_0\|\,. \qquad (6.57)\end{aligned}$$

Notice that in the approximate solution of the full Schrödinger equation the state of the field is, up to a fast oscillating global phase $\mathrm{e}^{-\mathrm{i}e_0 t/\varepsilon}$, adiabatically following the motion of the particles. In particular, there are no bosons travelling back and forth between the particles and the phrase that the particles "interact through the exchange of bosons", which comes from perturbation theory, should not be taken literally in the present setting.

Let us stress the physical relevance of the allowed initial conditions in our result. Heuristically one would expect that *any* initial state for the Nelson model radiates its free bosons to infinity and thus effectively becomes a state in $\mathrm{Ran}P_*$. To make even precise this statement is not completely trivial and it is a hard problem in scattering theory to prove it. In case of the Nelson model for a single particle and with an infrared cutoff in the interaction, asymptotic completeness for Compton scattering was proven only recently in [FGS]. In particular, for a single particle the heuristic expectation formulated above holds true and every initial state, after a sufficiently long time, follows the effective dynamics.

As mentioned before, there is a strong similarity to the time-dependent Born-Oppenheimer approximation, where we obtained an effective Schrödinger equation for the nuclei in a molecule with an effective potential generated by the electrons in Section 2.3. In both cases the physical mechanism which leads to the approximate invariance of the subspace $\mathrm{Ran}P_*$ is adiabatic decoupling. I.e. the separation of time scales for the motion of the different parts of the system lets the fast degrees of freedom, in our case the bosons, instantaneously adjust to the motion of the slow degrees of freedom, the particles.

However, for massless bosons – in contrast to the Born-Oppenheimer approximation – there is no spectral gap which pointwise separates the energy band $E_0 = \{(x, E_0(x)) : x \in \mathbb{R}^{3N}\}$ from the remainder of the spectrum of $H_0(x)$, but E_0 lies at the bottom of continuous spectrum. Hence we need to apply the space-adiabatic theorem without gap, Theorem 6.3.

We emphasize at this point that, in view of the missing gap condition, the rate of convergence $\mathcal{O}(\varepsilon\sqrt{\ln(1/\varepsilon)})$ in (6.57) is surprisingly fast, since it is almost as good as in the case with a gap. Moreover, if all particles have individually total charge equal to zero, then the rate is exactly $\mathcal{O}(\varepsilon)$ as in the case with a gap. Hence, the logarithmic correction must be attributed to the Coulombic long range character of the interparticle interaction.

In contrast to the situation with gap, however, we do not expect that adiabatic decoupling holds to any order in ε. To the contrary, we expect that a piece of order ε^α, $\alpha < \infty$, of the wave function is "leaking out" of $P_*\mathcal{H}$. Physical considerations suggest that $\alpha = 3/2$ for the present problem, see Remark 6.12. As a consequence, the ε^2 corrections to the effective Hamiltonian are still dominating dissipation and can be formally derived from the results of Section 3.3. The effective Hamiltonian (6.67) then contains a renormalized mass term and the momentum dependent Darwin interaction.

We remark that in [AvEl$_2$] the time-adiabatic theorem without gap condition was applied to the Dicke model with a constant magnetic field whose direction changes slowly in time. The Dicke model is a simplified version of the spin-boson model, i.e. a two-level system coupled to the quantized massless scalar field. In the Dicke model one drops the anti-resonant terms in the interaction and can, as a consequence, explicitly calculate the ground state as a function of time. This is very similar to our setting, where we will obtain a rather explicit expression for the ground state of $H_0(x)$ as a function of $x \in \mathbb{R}^{3N}$. In [AvEl$_2$] the order of the error in the adiabatic limit is $\mathcal{O}(\varepsilon\sqrt{\ln(1/\varepsilon)})$, exactly as in (6.57). As to be explained, in both cases the specific form of the error can be traced back to the spectral density of the massless scalar field at zero energy.

Finally let us compare our results to those obtained by Davies [Da], who considers the limit $c \to \infty$ for the Hamiltonian

$$H^c = H_\mathrm{p} \otimes \mathbf{1} + \mathbf{1} \otimes \mathrm{d}\Gamma(c|k|) + \sqrt{c} H_\mathrm{I}\,.$$

Notice that H^c is obtained through canonical quantization of (6.41) and (6.42) if one does not set $c = 1$ as we did before. Davies proves that for all $t \in \mathbb{R}$

$$\mathrm{s} - \lim_{c\to\infty} \mathrm{e}^{-\mathrm{i}H^c t}(\psi \otimes \Omega) = (\mathrm{e}^{-\mathrm{i}(H_\mathrm{eff}+e_0)t}\psi) \otimes \Omega\,,$$

where $\Omega = \{1, 0, 0, \ldots\}$ denotes the Fock vacuum and $H_\mathrm{p} := H_\mathrm{p}^{\varepsilon=1}$ and $H_\mathrm{eff} := H_\mathrm{eff}^{\varepsilon=1}$. This shows that although the limit $c \to \infty$ is equivalent to our scaling on the classical level, the results for the quantum model differ qualitatively. While we obtain effective dynamics for states which contain a nonzero number of bosons independent of ε, cf. (6.57), the $c \to \infty$ limit yields effective dynamics for states which contain no bosons at all. Furthermore, the limit $\varepsilon \to 0$ is a singular limit as no limiting dynamics for $\varepsilon = 0$ exists. We thus encounter a situation similar to the one of constrained motion as discussed in Section 2.4.

6.3.2 Mathematical results

We now introduce the Nelson model in more detail. As explained, we consider N spinless particles coupled to a scalar, massless, Bose field with an ultraviolet regularization in the interaction. This class of models is nowadays called Nelson's model [Ar, Bz, LMS$_1$, LMS$_2$] after Nelson [Ne], who studied the ultraviolet problem. We briefly complete the introduction of the model and collect some basic, well known facts.

A point in the configuration space $\mathbb{R}^{3N}$ of the particles is denoted by $x = (x_1, \dots, x_N)$ and the Hamiltonian $H_{\mathrm{p}}^{\varepsilon}$ for the particles is defined in (6.45). $H_{\mathrm{p}}^{\varepsilon}$ is self-adjoint on the domain $H^1(\mathbb{R}^{3N})$, the first Sobolev space.

The Hilbert space for the scalar field is the bosonic Fock space over $L^2(\mathbb{R}^3)$ defined in (6.46). On $D(\sqrt{\mathcal{N}})$, $\mathcal{N}$ the number operator, the annihilation operator $a(f)$ acts for $f \in L^2(\mathbb{R}^3)$ as

$$(a(f)\psi)^{(m)}(k_1, \dots, k_m) = \sqrt{m+1} \int_{\mathbb{R}^3} \mathrm{d}k\, \bar{f}(k)\, \psi^{(m+1)}(k, k_1, \dots, k_m)\,,$$

where $\psi = (\psi^{(0)}, \psi^{(1)}, \psi^{(2)}, \dots) \in D(\sqrt{\mathcal{N}})$ if and only if $\sum_{m=0}^{\infty} m \|\psi^{(m)}\|^2 < \infty$. The adjoint $a^*(f)$, which is also defined on $D(\sqrt{\mathcal{N}})$, is the creation operator and for $f, g \in L^2(\mathbb{R}^3)$ the operators $a(f)$ and $a^*(g)$ obey the canonical commutation relations (CCRs)

$$[a(f), a^*(g)] = \int_{\mathbb{R}^3} \mathrm{d}k\, \bar{f}(k)\, g(k) =: \langle f, g \rangle\,, \quad [a(f), a(g)] = [a^*(f), a^*(g)] = 0\,. \tag{6.58}$$

It is common to write $a(f) = \int_{\mathbb{R}^3} dk\, \bar{f}(k)\, a(k)$. The Hamiltonian of the field as defined in (6.47) can formally be written as

$$H_{\mathrm{f}} = \int_{\mathbb{R}^3} \mathrm{d}k\, |k|\, a^*(k)\, a(k)\,.$$

More explicitly, on the m-particle sector the action of H_{f} is

$$(H_{\mathrm{f}}\psi)^{(m)}(k_1, \dots, k_m) = \sum_{j=1}^{m} |k_j| \psi^{(m)}(k_1, \dots, k_m)\,,$$

and H_{f} is self-adjoint on its maximal domain. For $f \in L^2(\mathbb{R}^3)$ the Segal field operator

$$\Phi(f) = \frac{1}{\sqrt{2}} \Big(a(f) + a^*(f) \Big)$$

is essentially self-adjoint on $D(\sqrt{\mathcal{N}})$. The field operator ϕ as used in (6.48) is related to Φ through $\phi(f) = \Phi(f/\sqrt{|k|})$. For the following it turns out to be more convenient to write the interaction Hamiltonian in terms of Φ, where

$$H_{\mathrm{I}} = \Phi\Big(|k|\, v(x, k) \Big)$$

acts on the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^{3N}) \otimes \mathcal{F}$ of the full system. We will consider two different choices for $v(x,k)$ in more detail. For the standard Nelson model (SN), as discussed in the previous section, one has

$$v_{\mathrm{SN}}(x,k) = \sum_{j=1}^{N} \mathrm{e}^{\mathrm{i}k\cdot x_j} \frac{\hat{\rho}_j(k)}{|k|^{3/2}} \,. \tag{6.59}$$

For the infrared-renormalized models (IR), as considered by Arai [Ar] and, more generally, by Lörinczi, Minlos and Spohn [LMS$_2$], one has

$$v_{\mathrm{IR}}(x,k) = \sum_{j=1}^{N} \left(\mathrm{e}^{\mathrm{i}k\cdot x_j} - 1\right) \frac{\hat{\rho}_j(k)}{|k|^{3/2}} \,. \tag{6.60}$$

In both cases, the charge distribution $\rho_j \in L^1(\mathbb{R}^3)$ of the j^{th} particle is assumed to be real-valued and spherically symmetric. As to be discussed below, cf. Remarks 6.7 and 6.9, we have to assume the infrared condition (6.49) for the (SN) model, but *not* for the (IR) model. The infrared condition implies, in particular, that the total charge of the system of N particles must be zero.

The full Hamiltonian is given as the sum

$$H^{\varepsilon} = H_{\mathrm{p}}^{\varepsilon} \otimes \mathbf{1} + \mathbf{1} \otimes H_{\mathrm{f}} + H_{\mathrm{I}} + V_{\mathrm{IR}} \otimes \mathbf{1} \tag{6.61}$$

and is essentially self-adjoint on $D(H_{\mathrm{p}} \otimes \mathbf{1}) \cap D(\mathbf{1} \otimes H_{\mathrm{f}})$ if for $s \in \{\frac{1}{2}, 1\}$ one has $\sup_x \| \, |k|^s v(x,k) \, \|_{L^2(\mathbb{R}^3)} < \infty$. *Only* in the (IR) model a potential V_{IR} is added, which acts as multiplication with the bounded, real-valued function

$$V_{\mathrm{IR}}(x) = \sum_{j,i=1}^{N} \int_{\mathbb{R}^3} \mathrm{d}k \, \frac{\hat{\rho}_j(k)\hat{\rho}_i(k)^*}{|k|^2} \, \mathrm{e}^{-\mathrm{i}k\cdot x_j} + \frac{1}{2} \int_{\mathbb{R}^3} \mathrm{d}k \, \left| \frac{\sum_{j=1}^{N} \hat{\rho}_j(k)}{|k|} \right|^2 \,. \tag{6.62}$$

Remark 6.7. If the charge distributions satisfy the infrared condition (6.49), then the (SN) Hamiltonian and the (IR) Hamiltonian are related by the unitary transformation

$$U_{\mathrm{G}} = \exp\left(-\mathrm{i}\Phi\left(\mathrm{i} \sum_{j=1}^{N} \frac{\hat{\rho}_j^*(k)}{|k|^{3/2}} \right) \right) \,,$$

cf. [Ar], which is related to the Gross transformation [Ne] for $x = 0$. If the infrared condition is not satisfied, the (SN) model and the (IR) model carry two inequivalent representations of the CCRs for the field operators. Physically speaking, the transformation U_{G} removes the mean field that the N charges would generate, if all of them would be moved to the origin. The vacuum in the (IR) representation corresponds to this removed mean field in the original representation, a fact which has to be taken care of in the

interaction: for each particle the interaction term is now evaluated relative to the interaction at $x = 0$, cf. (6.60), which makes also necessary the counter terms V_{IR}. If the total charge of the system is different from zero, then the mean field is long range and, as a consequence, the corresponding transformation is no longer unitarily implementable. Indeed, it was shown that the (SN) Hamiltonian with confining potential does *not* have a ground state, cf. [LMS$_2$], while the (IR) Hamiltonian with the same confining potential does have a ground state, cf. [Ar]. ♢

In order to apply Theorem 6.3 we observe that $H_{\mathrm{I}}(x)$ acts for fixed $x \in \mathbb{R}^{3N}$ ($\cong M$) on $\mathcal{F}$ ($\cong \mathcal{H}_{\mathrm{f}}$) and with $H_0(x) = H_{\mathrm{f}} + H_{\mathrm{I}}(x) + V_{\mathrm{IR}}(x)$ we have

$$H^\varepsilon = H_{\mathrm{p}}^\varepsilon \otimes \mathbf{1} + \int_M^\oplus \mathrm{d}x\, H_0(x) \quad \Big(\cong h^\varepsilon + H_0 \Big).$$

The following proposition collects some results about $H_0(x)$ and its ground state. Its proof is postponed to after the presentation of the the main theorem.

Proposition 6.8. *Assume that $v(x,\cdot) \in L^2(\mathbb{R}^3)$ for all $x \in \mathbb{R}^{3N}$ and that for some $n \geq 1$*

(i) $|\cdot|\partial_x^\alpha v(x,\cdot) \in L^2(\mathbb{R}^3)$ *for all* $x \in \mathbb{R}^{3N}$ *and* $0 \leq |\alpha| \leq n$,
(ii) $\sup_{x\in\mathbb{R}^{3N}} \| \sqrt{|\cdot|}\, \partial_x^\alpha v(x,\cdot) \|_{L^2(\mathbb{R}^3)} < \infty$ *for* $0 \leq |\alpha| \leq n$,
(iii) $\sup_{x\in\mathbb{R}^{3N}} \| \partial_x^\alpha v(x,\cdot) \|_{L^2(\mathbb{R}^3)} < \infty$ *for* $1 \leq |\alpha| \leq n$.

Let $\mathrm{Im}\langle v(x,\cdot), \nabla_x v(x,\cdot)\rangle_{L^2(\mathbb{R}^3)} = 0$ *for all* $x \in \mathbb{R}^{3N}$ *and* $V_{\mathrm{IR}}(\cdot) \in C_{\mathrm{b}}^3(\mathbb{R}^{3N})$. *Then*

1. *$H_0(x)$ is self adjoint on $\mathcal{D} = D(H_{\mathrm{f}})$ for all $x \in \mathbb{R}^{3N}$ and $H_0(\cdot) \in C_{\mathrm{b}}^n(\mathbb{R}^{3N}, \mathcal{L}(\mathcal{D},\mathcal{F}))$, where $\mathcal{D}$ is equipped with the graph-norm of H_{f}.*
2. *$H_0(x)$ has a unique ground state $\Omega(x)$ for all $x \in \mathbb{R}^{3N}$ and, in particular, $H_0(x)\Omega(x) = E(x)\Omega(x)$ for*

$$E(x) = -\frac{1}{2}\int_{\mathbb{R}^3} \mathrm{d}k\, |k|\, |v(x,k)|^2 + V_{\mathrm{IR}}(x). \tag{6.63}$$

Furthermore $\Omega(\cdot) \in C_{\mathrm{b}}^n(\mathbb{R}^{3N}, \mathcal{F})$.

It is straightforward to check that $\mathrm{Im}\langle v(x,\cdot), \nabla_x v(x,\cdot)\rangle_{L^2(\mathbb{R}^3)} = 0$ for v_{SN} defined in (6.59) and v_{IR} defined in (6.60). For the (SN) model as well as for the (IR) model (6.63) is easily evaluated and one finds $E(x) = E_0(x)$ as given in (6.53).

Remark 6.9. For the (SN) model the assumptions made on $v(x,k)$ in Proposition 6.8 are satisfied, if $\hat{\rho}_j(k)$ decays sufficiently fast for large $|k|$ and each $j = 1,\ldots,N$, or, equivalently, if $\rho_j(x)$ is sufficiently smooth. This is an ultraviolet condition individually for each particle. But $v(x,\cdot) \in L^2(\mathbb{R}^3)$ follows from $v(0,\cdot) \in L^2(\mathbb{R}^3)$, which is exactly the global infrared condition (6.49).

While the necessity for an ultraviolet regularization remains in the (IR) model, the infrared condition is replaced by $\sum_j |k|^{-\frac{3}{2}} \widehat{\rho}_j(k)(\mathrm{e}^{\mathrm{i}k\cdot x_j} - 1) \in L^2(\mathbb{R}^3)$, which can be satisfied without having $\sum_j \widehat{\rho}_j(0) = 0$. Thus the (IR) model allows us to consider particles with total charge different from zero. $\diamondsuit$

Let $P_*(x) = |\Omega(x)\rangle\langle\Omega(x)|$, then $P_*(\cdot) \in C^n_{\mathrm{b}}(\mathbb{R}^{3N}, \mathcal{L}(\mathcal{F}))$ and $P_*\mathcal{H}$ is a candidate for an adiabatically decoupled subspace. Indeed, we will show that $h^\varepsilon = H^\varepsilon_{\mathrm{p}} \otimes \mathbf{1}$ satisfies Condition $\mathbf{h}^m$ with $(Dh)^\varepsilon_{x_j} = -\mathrm{i}\varepsilon\nabla_{x_j}/\sqrt{-\varepsilon^2\Delta_{x_j} + 1}$ and that H_0 and P_* satisfy Assumption $\mathbf{H}^m_0$ (iii) with $\eta(\delta) = \delta\sqrt{\ln(1/\delta)}$ if particles with charges different from zero are present and $\eta(\delta) = \delta$ if all particles have total charge zero. Hence we can apply Theorem 6.3 to conclude that for some constant $C < \infty$

$$\left\| \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} - \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{diag}} t/\varepsilon} \right\| \leq C\,\eta(\varepsilon)\,(1 + |t|)\,, \tag{6.64}$$

with $H^\varepsilon_{\mathrm{diag}} = P_*\,H^\varepsilon\,P_* + (\mathbf{1} - P_*)\,H^\varepsilon\,(\mathbf{1} - P_*)$.

Next observe that the ground state band subspace $P_*\mathcal{H}$ is unitarily equivalent to the Hilbert space $L^2(\mathbb{R}^{3N})$ of the N particles in a natural way. Let

$$\mathcal{U} : P_*\mathcal{H} \to L^2(\mathbb{R}^{3N})\,, \quad \psi \mapsto (\mathcal{U}\psi)(x) = \langle \Omega(x), \psi(x)\rangle_{\mathcal{F}}\,, \tag{6.65}$$

then it is easily checked that for $\varphi \in L^2(\mathbb{R}^{3N})$

$$\mathcal{U}^*\varphi = \mathcal{U}^{-1}\varphi = \int_{\mathbb{R}^{3N}}^{\oplus} \mathrm{d}x\,\varphi(x)\,\Omega(x)\,.$$

Hence the part of $H^\varepsilon_{\mathrm{diag}}$ acting on $P_*\mathcal{H}$ is unitarily equivalent to

$$\widetilde{H}^\varepsilon_{\mathrm{eff}} = \mathcal{U}\,P_*\,H^\varepsilon\,P_*\,\mathcal{U}^*$$

acting on the Hilbert space of the N particles *only*. The following theorem shows that $\widetilde{H}^\varepsilon_{\mathrm{eff}}$ has, at leading order, exactly the form expected from the heuristic "Peierls substitution" argument.

Theorem 6.10. *Let H^ε be defined as in (6.61) with $v(x,k)$ either $v_{\mathrm{SN}}(x,k)$ as in (6.59) or $v_{\mathrm{IR}}(x,k)$ as in (6.60). For $1 \leq j \leq N$ let $\rho_j \in L^1(\mathbb{R}^3)$ such that $\hat{\rho}_j$ satisfies $|k|^s\widehat{\rho}_j(k) \in L^2(\mathbb{R}^3)$ for $s \in \{-1, 4\}$. For the (SN) model assume, in addition, the infrared condition (6.49). Let*

$$H^\varepsilon_{\mathrm{eff}} = H^\varepsilon_{\mathrm{p}} + \sum_{j=2}^{N}\sum_{i=1}^{j-1} V_{ij}(x_i - x_j) + e_0\,,$$

with $V_{ij}(z)$ and e_0 as in (6.54) and (6.55). Then there is a constant $C < \infty$ such that

$$\left\| \left(\mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} - \mathcal{U}^*\,\mathrm{e}^{-\mathrm{i}H^\varepsilon_{\mathrm{eff}} t/\varepsilon}\,\mathcal{U} \right) P_* \right\| \leq C\,\eta(\varepsilon)\,(1 + |t|)\,, \tag{6.66}$$

where $\eta(\varepsilon) = \varepsilon\sqrt{\ln(1/\varepsilon)}$. If all charges satisfy the infrared condition individually, i.e. if $\hat{\rho}_j(k)/|k|^{3/2} \in L^2(\mathbb{R}^3)$ for all $j = 1, \ldots, N$, then (6.66) holds with $\eta(\varepsilon) = \varepsilon$.

For sake of better readability the global energy shift e_0 was, as opposed to (6.57), absorbed into the definition of $H^\varepsilon_{\rm eff}$.

Remark 6.11. Exactly as in the adiabatic theory with gap we have the following important property of the effective dynamics. The unitary $\mathcal{U}$ intertwines the position operator $x \otimes \mathbf{1}$ on $L^2(\mathbb{R}^{3N}) \otimes \mathcal{F}$ with the position operator x on $L^2(\mathbb{R}^{3N})$ exactly and the momentum operator $-\mathrm{i}\varepsilon\nabla_x \otimes \mathbf{1}$ on $L^2(\mathbb{R}^{3N}) \otimes \mathcal{F}$ with $-\mathrm{i}\varepsilon\nabla_x$ on $L^2(\mathbb{R}^{3N})$ up to an error of order ε. Thus one can directly read off the position distribution and approximately also the momentum distribution of the particles from the solution $\psi(t) = \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm eff}t/\varepsilon}\psi_0$ of the effective dynamics. It is *not* necessary to transform back to the full Hilbert space using $\mathcal{U}^*$. ♢

Remark 6.12. From the discussion of Section 6.3.1 one expects, on physical grounds, that the energy lost through radiation is of order $\mathcal{O}(\varepsilon^3)$ after times of order $\mathcal{O}(\varepsilon^{-1})$. Hence the error of order $\mathcal{O}(\varepsilon\sqrt{\ln 1/\varepsilon})$ in (6.66) is not optimal in the sense that the error does not correspond to emission of free bosons and thus to dissipation. Indeed, we expect that the situation is similar to adiabatic perturbation theory with gap, cf. Chapter 3. There should be a subspace $P^\varepsilon_*\mathcal{H}$ which is ε-close to $P_*\mathcal{H}$ and for which the analogous expression to (6.64) holds with an error of order $\mathcal{O}(\varepsilon^{\frac{3}{2}})$, possibly with a logarithmic correction. The corresponding effective Hamiltonian would then contain two additional terms of order ε^2, which, for the case of quadratic dispersion

$$H^\varepsilon_{\rm p} = -\sum_{j=1}^N \frac{\varepsilon^2}{2}\Delta_{x_j}$$

for the particles, can be calculated using formula (4.35). As result we obtain for the Weyl symbol of the effective Hamiltonian including the momentum dependent Darwin term

$$\begin{aligned} H_{\rm eff}(p,q) = &\sum_{j=1}^N \frac{1}{2m^\varepsilon_j}\, p_j^2 + E(q) \\ &+ \frac{\varepsilon^2}{2}\sum_{j<i}\int_{\mathbb{R}^3} \mathrm{d}k\, \frac{(p_j\cdot\kappa)(p_i\cdot\kappa)}{|k|^2}\mathrm{e}^{-\mathrm{i}k\cdot(q_j-q_i)}\hat\rho^*_j(k)\hat\rho_i(k) \end{aligned} \tag{6.67}$$

with $m^\varepsilon_j = 1/(1+\frac{\varepsilon^2}{2}e_j)$ and

$$e_j = \frac{1}{4\pi}\int_{\mathbb{R}^3\times\mathbb{R}^3} \mathrm{d}v\,\mathrm{d}w\,\frac{\rho_j(v)\rho_j(w)}{|v-w|}$$

the electromagnetic mass. As explained above, for the rigorous justification of (6.67) a space-adiabatic theorem without gap but for rotated subspaces P^ε_* is needed. ♢

Before proving Theorem 6.10 we make up for the

Proof (of Proposition 6.8). A standard estimate (cf. e.g. [Bz] Proposition 1.3.8) shows that for $f \in L^2(\mathbb{R}^3)$ and any $a > 0$

$$\|\Phi(f)\psi\|_{\mathcal{F}}^2 \leq a\|H_{\mathrm{f}}\psi\|_{\mathcal{F}}^2 + \left(\frac{\|f/\sqrt{|\cdot|}\,\|_{L^2(\mathbb{R}^3)}^4}{a} + 2\right)\|\psi\|_{\mathcal{F}}^2 . \tag{6.68}$$

Hence $\Phi(f)$ is infinitesimally H_{f}-bounded whenever

$$\|f\|_{L^2(\mathbb{R}^3)} + \|f/\sqrt{|\cdot|}\,\|_{L^2(\mathbb{R}^3)} < \infty .$$

Then Kato-Rellich implies that $H_0(x)$ is self-adjoint on $D(H_{\mathrm{f}})$, since by assumption we have $\sqrt{|\cdot|}v(x,\cdot) \in L^2$. Using (i), (ii) and $V_{\mathrm{IR}}(\cdot) \in C_{\mathrm{b}}^n(\mathbb{R}^{3N})$, we obtain from (6.68) that

$$\partial_x^\alpha H_0(x) = \Phi\left(|k|\,\partial_x^\alpha v(x,k)\right) + \partial_x^\alpha V_{\mathrm{IR}}(x) \tag{6.69}$$

is relatively bounded with respect to H_{f} for $|\alpha| \leq n$. Moreover, (ii), (6.68) and (6.69) imply that $H_0(\cdot) \in C_{\mathrm{b}}^n(\mathbb{R}^{3N}, \mathcal{L}(\mathcal{D},\mathcal{F}))$.

To compute the ground state energy $E(x)$ observe that from "completing the square" one finds

$$\begin{aligned} H_0(x) = &\int_{\mathbb{R}^3} \mathrm{d}k\,|k| \left(a^*(k) + \frac{v^*(k,x)}{\sqrt{2}}\right)\left(a(k) + \frac{v(x,k)}{\sqrt{2}}\right) \\ &- \frac{1}{2}\int_{\mathbb{R}^3} \mathrm{d}k\,|k|\,|v(x,k)|^2 + V_{\mathrm{IR}}(x) . \end{aligned}$$

It is well known that the map $a(k) \mapsto a(k) + v(x,k)/\sqrt{2}$ comes from the unitary transformation $U(x) = \exp\left(\mathrm{i}\Phi\big(\mathrm{i}v(x,\cdot)\big)\right)$, i.e.

$$U(x)\,a(f)\,U^*(x) = a(f) + \langle f, v(x,\cdot)\rangle , \tag{6.70}$$

whenever $v(x,\cdot) \in L^2$. Equation (6.70) follows from the fact that $[A,[A,B]] = 0$ implies $[\exp(\mathrm{i}A), B] = \exp(\mathrm{i}A)[\mathrm{i}A, B]$ and the CCRs. Transformations of the form (6.70) are called Bogoliubov transformations.

Therefore $H_0(x) = U(x)\,H_{\mathrm{f}}\,U^*(x) + E(x)$ with

$$E(x) = -\frac{1}{2}\int_{\mathbb{R}^3} \mathrm{d}k\,|k|\,|v(x,k)|^2 + V_{\mathrm{IR}}(x) .$$

Since $H_{\mathrm{f}}\,\Omega_0 = 0$ for the unique ground state $\Omega_0 = (1,0,0,\ldots) \in \mathcal{F}$, we find

$$H_0(x)\Omega(x) = E(x)\Omega(x) \quad \text{with} \quad \Omega(x) = U(x)\Omega_0 .$$

Next we need to take derivatives of $U(x)$ with respect to x. It follows from the CCRs (6.58) that for $f, g \in L^2(\mathbb{R}^3)$

$$\big[\Phi(f),\Phi(g)\big] = \mathrm{i}\,\mathrm{Im}\langle f,g\rangle\,,$$

and thus, by assumption, that $\nabla_x\Phi(\mathrm{i}v(\cdot,x)) = \Phi(\mathrm{i}\nabla_x v(\cdot,x))$ commutes with $\Phi(\mathrm{i}v(\cdot,x))$. Hence we obtain that on $D(\sqrt{\mathcal{N}})$

$$\nabla_x U(x) = U(x)\,\mathrm{i}\Phi(\mathrm{i}\nabla_x v(\cdot,x)) = \mathrm{i}\Phi(\mathrm{i}\nabla_x v(\cdot,x))\,U(x)\,. \tag{6.71}$$

By further differentiating (6.71) we can get up to n^{th} derivatives since $\partial_x^\alpha v(x,k) \in L^2(\mathbb{R}^3)$ for $|\alpha| \leq n$. In particular we find with (iii) that $\Omega(x) = U(x)\Omega_0 \in C^n_{\mathrm{b}}(\mathbb{R}^{3N},\mathcal{F})$. □

Proof (of Theorem 6.10). We start by showing that the assumptions of Theorem 6.3 are indeed satisfied and thus (6.64) follows.

It is straightforward to check that the assumptions on $\hat\rho_j$ imply the assumptions of Proposition 6.8 for $n = 5$. Hence the first part of $\mathbf{H}^4_0$ follows with $P_*(x) = |\Omega(x)\rangle\langle\Omega(x)|$. For $\mathbf{H}^4_0$ (iii) observe that, using (6.71), $\nabla_x\Omega(x) = \nabla_x U(x)\Omega_0 = U(x)\,\mathrm{i}\Phi(\mathrm{i}\nabla_x v(\cdot,x))\Omega_0$, and thus

$$\langle\Omega(x),\nabla_x\Omega(x)\rangle_{\mathcal{F}} = \langle\Omega_0,\mathrm{i}\Phi(\mathrm{i}\nabla_x v(\cdot,x))\Omega_0\rangle_{\mathcal{F}} = 0\,. \tag{6.72}$$

As a consequence, $(\nabla_x P_*)(x)P_*(x) = |\nabla_x\Omega(x)\rangle\langle\Omega(x)|$. Hence we obtain for $1 \leq j \leq N$

$$R(\delta,x)(\nabla_{x_j}P_*)(x)P_*(x) = i\,|U(x)\,R_{\mathrm{f}}(\delta)\,\Phi(\mathrm{i}\nabla_{x_j}v(\cdot,x))\Omega_0\rangle\langle\Omega(x)|\,, \tag{6.73}$$

where $R_{\mathrm{f}}(\delta) = (H_{\mathrm{f}} - \mathrm{i}\delta)^{-1}$. For (6.15) one therefore finds

$$\begin{aligned}\|R(\delta,x)(\nabla_{x_j}P_*)(x)P_*(x)\|^2_{\mathcal{L}(\mathcal{F})} &= \|R_{\mathrm{f}}(\delta)\Phi(\mathrm{i}\nabla_{x_j}v(x,\cdot))\Omega_0\|^2_{\mathcal{F}} \\ &= \Big\|(|k| - \mathrm{i}\delta)^{-1}k\,\mathrm{e}^{\mathrm{i}k\cdot x_j}\hat\rho_j(k)|k|^{-\frac{3}{2}}\Big\|^2_{L^2(\mathbb{R}^3)}\end{aligned} \tag{6.74}$$

Whenever ρ_j satisfies the infrared condition $\hat\rho_j(k)|k|^{-\frac{3}{2}} \in L^2(\mathbb{R}^3)$, (6.75) is bounded uniformly in δ since $\big|\,|k|/(|k| - \mathrm{i}\delta)\,\big| \leq 1$. In general we only assume that $\hat\rho_j(k)|k|^{-1} \in L^2(\mathbb{R}^3)$. Using that $\hat\rho_j(k)$ is bounded uniformly according to Riemann-Lebesgue, (6.75) becomes

$$\begin{aligned}\Big\|(|k| - \mathrm{i}\delta)^{-1}k\,\mathrm{e}^{\mathrm{i}k\cdot x_j}\hat\rho_j(k)|k|^{-\frac{3}{2}}\Big\|^2_{L^2(\mathbb{R}^3)} &\leq C_1\int_0^1 \mathrm{d}|k|\frac{|k|}{|k|^2+\delta^2} + C_2 \\ &\leq C\ln 1/\delta\,,\end{aligned} \tag{6.75}$$

for $\delta \in (0,\frac{1}{2}]$. To obtain the estimate (6.16), we differentiate (6.73) and find

$$\begin{aligned}\nabla_{x_i}\Big(R(\delta,x)(\nabla_{x_j}P_*)(x)P_*(x)\Big) &= \mathrm{i}\,|U(x)\,R_{\mathrm{f}}(\delta)\Phi(\mathrm{i}\nabla_{x_j}v(x,\cdot))\Omega_0\rangle\langle\nabla_{x_i}\Omega(x)| \\ &\quad - |U(x)\,\Phi(\mathrm{i}\nabla_{x_i}v(x,\cdot))\,R_{\mathrm{f}}(\delta)\Phi(\mathrm{i}\nabla_{x_j}v(x,\cdot))\Omega_0\rangle\langle\Omega(x)| \\ &\quad + \mathrm{i}\,|U(x)\,R_{\mathrm{f}}(\delta)\Phi(\mathrm{i}\nabla^{(2)}_{ij}v(x,\cdot))\Omega_0\rangle\langle\Omega(x)|\,.\end{aligned} \tag{6.76}$$

All three terms in (6.76) can be bounded by using the same type of arguments as in (6.75) and (6.75): For the first term use in addition that $\|\nabla_{x_i}\Omega(x)\|_{\mathcal{H}_\mathrm{f}} < C$ and for the second term one has to estimate the components in the 0-boson sector and in the 2-boson sector separately. In summary we showed that $\mathbf{H}_0^4$ (iii) is satisfied with $\eta(\delta) = \delta\sqrt{\ln(1/\delta)}$, and with $\eta(\delta) = \delta$ if all charges satisfy the infrared condition individually.

We are left to check for Assumption $\mathbf{h}^4$. Let

$$h^\varepsilon = H_\mathrm{p}^\varepsilon \otimes \mathbf{1} = \sum_j h(-\mathrm{i}\varepsilon\nabla_{x_j}) \otimes \mathbf{1}\,,$$

with $h(p) = \sqrt{p^2+1}$. Essential self-adjointness of $h^\varepsilon + H_0$ on $D(H_\mathrm{p}\otimes\mathbf{1}) \cap D(H_0)$ is a standard result, cf. Proposition 2.1 in [Ar]. We define $(Dh)_j^\varepsilon = (\nabla h)(-\mathrm{i}\varepsilon\nabla_{x_j}) \otimes \mathbf{1}$, with $\|(Dh)^\varepsilon\|_{\mathcal{L}(\mathcal{H})^{\oplus 3N}} \leq 1$, and postpone the technical proof of the following Lemma to the end of this section.

Lemma 6.13. *h^ε and $(Dh)^\varepsilon$ satisfy $\mathbf{h}^4$ (i) and (ii).*

We conclude that all assumptions of Theorem 6.3 are satisfied for the (SN) and the (IR) model and thus (6.64) holds. However, (6.66) follows from (6.64) by the following Lemma and an argument like (6.21). □

Lemma 6.14. *There is a constant $C < \infty$ such that for $\varepsilon > 0$ sufficiently small*

$$\left\| \left(H_\mathrm{diag}^\varepsilon - \mathcal{U}^* H_\mathrm{eff}^\varepsilon \mathcal{U} \right) P_* \right\|_{\mathcal{L}(\mathcal{H})} \leq \varepsilon^2 C\,.$$

Proof. In order to apply $\mathbf{h}^4$ (i) to $\mathcal{U}(x)$, we have to extend $\mathcal{U}(x) : P_*(x)\mathcal{F} \to \mathbb{C}$ defined in (6.65) to a map $\widetilde{\mathcal{U}}(\cdot) \in C_\mathrm{b}^4(\mathbb{R}^{3N}, \mathcal{L}(\mathcal{F}))$ first. To this end let $\widetilde{\mathcal{U}}(x) = |\Omega_0\rangle\langle\Omega(x)|$ and note that $\widetilde{\mathcal{U}}^*\widetilde{\mathcal{U}} = P_*$. With this definition one finds

$$\begin{aligned} H_\mathrm{diag}^\varepsilon P_* &= H_0 P_* + P_* h^\varepsilon P_* = E P_* + P_* \widetilde{\mathcal{U}}^* h^\varepsilon \widetilde{\mathcal{U}} P_* + P_* [h^\varepsilon, \widetilde{\mathcal{U}}^*] \widetilde{\mathcal{U}} P_* \\ &= \mathcal{U}^* H_\mathrm{eff}^\varepsilon \mathcal{U} P_* + P_* [h^\varepsilon, \widetilde{\mathcal{U}}^*] \widetilde{\mathcal{U}} P_*\,, \end{aligned}$$

and we are left to show that $\|P_* [h^\varepsilon, \widetilde{\mathcal{U}}^*] \widetilde{\mathcal{U}} P_*\| = \mathcal{O}(\varepsilon^2)$. Using $\mathbf{h}^4$ (i) with $A = \widetilde{\mathcal{U}}^*$ we find that

$$P_* [h^\varepsilon, \widetilde{\mathcal{U}}^*] \widetilde{\mathcal{U}} P_* = -\mathrm{i}\varepsilon P_* (\nabla_x \widetilde{\mathcal{U}}^*) \cdot (Dh)^\varepsilon \widetilde{\mathcal{U}} P_* + \mathcal{O}(\varepsilon^2)\,.$$

However, according to (6.72)

$$P_*(x)(\nabla_x \widetilde{\mathcal{U}}^*)(x) = |\Omega(x)\rangle\langle\Omega(x),\, \nabla_x \Omega(x)\rangle\langle\Omega_0| = 0\,,$$

and thus the desired result follows. □

Proof (of Lemma 6.13). Heuristically $\mathbf{h}^4$ (i) and (ii) hold, because they are just special cases of the expansion of a commutator of pseudodifferential operators. However, since h^ε is unbounded and A is only 4-times differentiable, we need to check the estimates "by hand".

For notational simplicity we restrict ourselves to the case $N = 1$, from which the general case follows immediately. Let $g(p) = 1/\sqrt{p^2+1}$, $g^\varepsilon = g(-\mathrm{i}\varepsilon\nabla_x) \otimes \mathbf{1}$ and $A \in C^4_{\mathrm{b}}(\mathbb{R}^3, \mathcal{H}_{\mathrm{f}})$, then $|\cdot|^s \widehat{g} \in L^1(\mathbb{R}^3)$ for $s \in \{0, 4\}$ and thus for $\psi \in \mathcal{S}$

$$
\begin{aligned}
&\Big(g^\varepsilon A\psi\Big)(x) = (2\pi)^{-\frac{3}{2}} \int \mathrm{d}y\, \widehat{g}(y)\, A(x-\varepsilon y)\, \psi(x-\varepsilon y) \\
&= \int \mathrm{d}y\, \widehat{g}(y) \left(A(x) - \varepsilon y \cdot \nabla A(x) + \varepsilon^2 \int_0^1 \mathrm{d}s \langle y, \nabla^{(2)} A(x - s\varepsilon y) y\rangle\right) \psi(x-\varepsilon y) \\
&= \Big(Ag^\varepsilon\psi\Big)(x) - \mathrm{i}\,\varepsilon\Big(\nabla A \cdot \nabla g^\varepsilon \psi\Big)(x) \\
&\qquad + (2\pi)^{-\frac{3}{2}} \int \mathrm{d}y\, \widehat{g}(y)\, \varepsilon^2 \int_0^1 \mathrm{d}s\, \langle y, \nabla^{(2)} A(x - s\varepsilon y)\, y\rangle \psi(x-\varepsilon y)\,. \qquad (6.77)
\end{aligned}
$$

From (6.77) one concludes after a lengthy but straightforward computation involving several integrations by parts that

$$
\varepsilon^2 \Delta_x\, [g^\varepsilon, A] = -\mathrm{i}\,\varepsilon \nabla A \cdot (\nabla g)^\varepsilon\, (\varepsilon^2 \Delta_x) + R
$$

with

$$
\|R\| \leq C \sum_{j=2}^{4} \varepsilon^j \sup_{x \in \mathbb{R}^{3N},\, |\alpha| = j} \|\partial_x^\alpha A(x)\|_{\mathcal{L}(\mathcal{H}_{\mathrm{f}})}\,.
$$

Hence we find

$$
\begin{aligned}
[h^\varepsilon, A] &= [(1-\varepsilon^2\Delta_x) g^\varepsilon, A] = (1-\varepsilon^2\Delta_x)[g^\varepsilon, A] - [\varepsilon^2\Delta_x, A] g^\varepsilon \\
&= -\mathrm{i}\,\varepsilon \nabla A \cdot (Dh)^\varepsilon + R'
\end{aligned}
$$

with

$$
\|R'\| \leq C' \sum_{j=2}^{4} \varepsilon^j \sup_{x \in \mathbb{R}^{3N},\, |\alpha| = j} \|\partial_x^\alpha A(x)\|_{\mathcal{L}(\mathcal{H}_{\mathrm{f}})}\,.
$$

This proves $\mathbf{h}^4$ (i). By the same type of arguments one shows also $\mathbf{h}^4$ (ii). □

A Pseudodifferential operators

In this appendix we review those aspects of pseudodifferential calculus with operator valued symbols, which are used in Chapter 3 and Chapter 4. As emphasized in many textbooks on pseudodifferential calculus, e.g. [Hö$_2$, Fo, DiSj], it is possible to generalize the theory for scalar valued symbols to large classes of operator valued symbols. For the convenience of the reader and to settle the notation, we provide a self-contained review of the basic results. For the proofs we mostly refer to Folland's book [Fo], because they all carry over from the scalar case to operator valued symbols with minor changes. We remark that a slightly different but equivalent formulation of pseudodifferential calculus with operator valued symbols is contained in the book of Dimassi and Sjöstrand [DiSj], based on an unpublished work of Balazard-Konlein [Ba].

A.1 Weyl quantization and symbol classes

Before entering the mathematics, recall that the basic idea of "quantization" is to turn functions on phase space $\mathbb{R}^{2d} = \mathbb{R}^d_q \times \mathbb{R}^d_p$ into operators acting on some space of functions over $\mathbb{R}^d_x$, in our case mostly $L^2(\mathbb{R}^d)$. The basic requirement is that the function $(q,p) \mapsto q$ is mapped into multiplication with x and the function $(q,p) \mapsto p$ is mapped to the differential operator $-\mathrm{i}\varepsilon\nabla_x$, where $\varepsilon > 0$ is some parameter for the moment. For functions $f(q,p) = g(q) + h(p)$ this rule is basically unique, since, as acting on $L^2(\mathbb{R}^d)$, the operators $g(x)$ and $h(-\mathrm{i}\varepsilon\nabla_x)$ are defined through the functional calculus for self-adjoint operators. For general functions the non-commutativity of x and $-\mathrm{i}\varepsilon\nabla_x$ makes a specific choice and a more careful definition necessary. In the following we adopt the Weyl-quantization rule, which, in particular, has the advantage that real-valued functions are mapped into self-adjoint operators. Notice however, that the fundamental Hamiltonians in physics which we consider in this monograph are all given uniquely, usually in the form of differential operators. Rewriting them as Weyl-quantizations is purely a convenient way to get the analysis started. There is no arbitrariness introduced here.

With the basic idea in mind we come to the mathematical definitions. Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be separable Hilbert spaces and denote by $\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$ the space

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of bounded linear operators from $\mathcal{H}_1$ to $\mathcal{H}_2$. Let A be a $\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$-valued rapidly decreasing smooth function on $\mathbb{R}^{2d}$, i.e. $A \in \mathcal{S}(\mathbb{R}^{2d}, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$. If we denote by $\mathcal{F}A$ the Fourier transform of A then, by Fourier inversion formula,

$$A(q,p) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} \mathrm{d}\eta \, \mathrm{d}\xi \, (\mathcal{F}A)(\eta,\xi) \, \mathrm{e}^{\mathrm{i}(\eta\cdot q + \xi\cdot p)} \,, \tag{A.1}$$

where the integral is a Bochner integral for $\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$-valued functions. With

$$L^2(\mathbb{R}^d, \mathcal{H}) \cong L^2(\mathbb{R}^d) \otimes \mathcal{H}$$

in mind, this suggest to define the operator

$$\widehat{A} : L^2(\mathbb{R}^d, \mathcal{H}_1) \to L^2(\mathbb{R}^d, \mathcal{H}_2)$$

called the **Weyl quantization** of the **symbol** A, by substituting in (A.1)

$$\mathrm{e}^{\mathrm{i}(\eta\cdot q + \xi\cdot p)} \to \mathrm{e}^{\mathrm{i}(\eta\cdot \widehat{q} + \xi\cdot \widehat{p})} \otimes \mathbf{1}_{\mathcal{H}_1} \,,$$

where $\widehat{q}$ is multiplication by x and $\widehat{p} = -\mathrm{i}\varepsilon\nabla_x$ in $L^2(\mathbb{R}^d)$. The exponential is defined by using the spectral theorem and it is explicitly given through

$$\left(\mathrm{e}^{\mathrm{i}(\eta\cdot \widehat{q} + \xi\cdot \widehat{p})} \, \psi \right)(x) = \mathrm{e}^{\mathrm{i}\varepsilon(\eta\cdot\xi)/2} \, \mathrm{e}^{\mathrm{i}\eta\cdot x} \, \psi(x + \varepsilon\xi) \qquad \text{for } \psi \in L^2(\mathbb{R}^d). \tag{A.2}$$

Thus

$$\widehat{A} = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} \mathrm{d}\eta \, \mathrm{d}\xi \; \mathrm{e}^{\mathrm{i}(\eta\cdot \widehat{q} + \xi\cdot \widehat{p})} \otimes (\mathcal{F}A)(\eta,\xi) \tag{A.3}$$

defines a bounded operator from $L^2(\mathbb{R}^d, \mathcal{H}_1)$ to $L^2(\mathbb{R}^d, \mathcal{H}_2)$ provided that the Fourier transform of A belongs to $L^1(\mathbb{R}^{2d}, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$. In particular,

$$\big\|\widehat{A}\big\|_{\mathcal{L}(L^2(\mathbb{R}^d,\mathcal{H}_1), L^2(\mathbb{R}^d,\mathcal{H}_2))} \leq \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} \mathrm{d}\eta \, \mathrm{d}\xi \; \|(\mathcal{F}A)(\eta,\xi)\|_{\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)} \,.$$

We also use the notation $\mathcal{W}_\varepsilon(A) \equiv \widehat{A}$ in order to emphasize the ε-dependence or if the expression for the symbol is too long to put a hat on it. Substituting (A.2) in (A.3) one obtains that for every $\psi \in \mathcal{S}(\mathbb{R}^d, \mathcal{H}_1)$

$$\big(\widehat{A}\psi\big)(x) = \frac{1}{(2\pi\varepsilon)^d} \int_{\mathbb{R}^{2d}} \mathrm{d}\xi \, \mathrm{d}y \, A\big(\tfrac{1}{2}(x+y), \xi\big) \, \mathrm{e}^{\mathrm{i}\xi\cdot(x-y)/\varepsilon} \, \psi(y) \,, \tag{A.4}$$

i.e. $\widehat{A}$ is an integral operator with kernel

$$K_A(x,y) = \frac{1}{(2\pi\varepsilon)^d} \int_{\mathbb{R}^d} \mathrm{d}\xi \, A\big(\tfrac{1}{2}(x+y), \xi\big) \; \mathrm{e}^{\mathrm{i}\xi\cdot(x-y)/\varepsilon} \,.$$

When applied to functions in $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_1)$, the expression (A.4) makes sense for a much larger class of symbols. There are basically two different types of classes of symbols, which have different advantages to work with. We shall make use of both types of symbol classes, which is the reason that the following definitions are somewhat lengthy.

We start with the "old" symbol classes, cf. [Hö$_2$, Fo], for which the pseudodifferential calculus was originally developed.

Definition A.1. *A function $A \in C^\infty(\mathbb{R}^{2d}, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ belongs to the symbol class $S^m_\rho(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ with $m \in \mathbb{R}$ and $0 \leq \rho \leq 1$, if for every $\alpha, \beta \in \mathbb{N}^d$ there exists a positive constant $C_{\alpha,\beta}$ such that*

$$\sup_{q \in \mathbb{R}^d} \left\| (\partial_q^\alpha \partial_p^\beta A)(q,p) \right\|_{\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)} \leq C_{\alpha,\beta} \, \langle p \rangle^{m-\rho|\beta|}$$

for every $p \in \mathbb{R}^d$, where $\langle p \rangle = (1 + |p|^2)^{1/2}$.

The space $S^m_\rho(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ is a Fréchet space, whose topology is defined by the (directed) family of semi-norms

$$\|A\|_k^{(m)} = \sup_{|\alpha|+|\beta| \leq k} \sup_{q,p \in \mathbb{R}^d} \langle p \rangle^{-m+\rho|\beta|} \left\| (\partial_q^\alpha \partial_p^\beta A)(q,p) \right\|_{\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)} , \quad k \in \mathbb{N} . \tag{A.5}$$

Functions in S^m_ρ with $\rho > 0$ have the nice property that every derivative with respect to p improves the decay with respect to p at infinity. This fact can be used to obtain asymptotic expansions of symbols with respect to the degree of decay in p. On the other hand, in the context of parameter dependent or semiclassical pseudodifferential calculus, cf. [DiSj, Ma$_1$], one has an additional parameter, e.g. $\hbar$ or, as in this monograph, ε, and asymptotic expansions are with respect to this parameter. As a consequence the symbol classes predominantly used in semiclassics have $\rho = 0$ and one allows for more general bounds than $\langle p \rangle^m$, called order functions.

Definition A.2. *A function $w : \mathbb{R}^{2d} \to [0, +\infty)$ is said to be an **order function** if there exist constants $C_0 > 0$ and $N_0 > 0$ such that*

$$w(x) \leq C_0 \, \langle x - y \rangle^{N_0} \, w(y)$$

for every $x, y \in \mathbb{R}^{2d}$.

It is obvious and will be used implicitly that the product of two order functions is again an order function.

Definition A.3. *A function $A \in C^\infty(\mathbb{R}^{2d}, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ belongs to the symbol class $S^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ with order function w, if for every $\alpha, \beta \in \mathbb{N}^d$ there exists a positive constant $C_{\alpha,\beta}$ such that*

$$\left\| (\partial_q^\alpha \partial_p^\beta A)(q,p) \right\|_{\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)} \leq C_{\alpha,\beta} \, w(q,p) \tag{A.6}$$

for every $q, p \in \mathbb{R}^d$.

Again the spaces $S^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ are Fréchet spaces with a family of semi-norms given through the minimal constants satisfying (A.6).

Clearly the functions $w(q,p) = \langle p \rangle^m$ are order functions and thus $S^m_0 = S^{w=\langle p \rangle^m}$.

The proof of the following result is a straightforward generalization of the corresponding result for scalar symbols, cf. Theorem 2.21 in [Fo] and Lemma 7.8 in [DiSj]. We reproduce the proof from [Fo] in order to convince the reader that nothing changes at this level when considering operator valued symbols.

Proposition A.4. *Let $A \in S^m_\rho(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$ or $A \in S^w(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$, then $\widehat{A}$ given through the uniformly convergent integral (A.4) defines a continuous mapping from $\mathcal{S}(\mathbb{R}^d,\mathcal{H}_1)$ to $\mathcal{S}(\mathbb{R}^d,\mathcal{H}_2)$.*

Proof. We give the proof for $A \in S^m_\rho(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$ and refer to Lemma 7.8 in [DiSj] for the statement for $A \in S^w(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$. Given $\psi \in \mathcal{S}(\mathbb{R}^d,\mathcal{H}_1)$, then

$$g(x,\xi) = \int_{\mathbb{R}^d} \mathrm{d}y\, A\big(\tfrac{1}{2}(x+y),\xi\big)\,\psi(y)\,\mathrm{e}^{\mathrm{i}\xi\cdot(x-y)/\varepsilon}$$

converges in norm in $\mathcal{H}_2$ as a Bochner integral. Substituting $u = y - x$ and abbreviating $L_u := -\varepsilon^2\Delta_u$, one finds that for any positive integer M

$$\begin{aligned}
g(x,\xi) &= \int_{\mathbb{R}^d} \mathrm{d}u\, A\big(x+\tfrac{1}{2}u,\xi\big)\,\psi(u+x)\,\mathrm{e}^{-\mathrm{i}\xi\cdot u/\varepsilon} \\
&= \int_{\mathbb{R}^d} \mathrm{d}u\, A\big(x+\tfrac{1}{2}u,\xi\big)\,\psi(u+x)\,\langle\xi\rangle^{-2M}\,(1+L_u)^M\,\mathrm{e}^{-\mathrm{i}\xi\cdot u/\varepsilon} \\
&= \int_{\mathbb{R}^d} \mathrm{d}u\, \frac{\mathrm{e}^{-\mathrm{i}\xi\cdot u/\varepsilon}}{\langle\xi\rangle^{2M}}\,(1+L_u)^M\,\big[A\big(x+\tfrac{1}{2}u,\xi\big)\,\psi(u+x)\big] \\
&= \sum_{|\alpha+\beta|\le 2M} c_{\alpha\beta} \int_{\mathbb{R}^d} \mathrm{d}u\, \frac{\mathrm{e}^{-\mathrm{i}\xi\cdot u/\varepsilon}}{\langle\xi\rangle^{2M}}\,\partial_x^\alpha A\big(x+\tfrac{1}{2}u,\xi\big)\,\partial_x^\beta\psi(u+x)\,.
\end{aligned}$$

Hence we have for arbitrary $M \in \mathbb{N}$ that

$$\begin{aligned}
\|g(x,\xi)\|_{\mathcal{H}_2} &\le C_M \sum_{|\alpha+\beta|\le 2M} \int_{\mathbb{R}^d} \mathrm{d}u\,\langle\xi\rangle^{-2M+m}\|\partial_x^\beta\psi(x+u)\|_{\mathcal{H}_1} \\
&\le C_M\langle\xi\rangle^{-2M+m}\underbrace{\int_{\mathbb{R}^d}\mathrm{d}u\,\|\partial_u^\beta\psi(u)\|_{\mathcal{H}_1}}_{=\,\|\partial^\beta\psi\|_{L^1(\mathbb{R}^d,\mathcal{H}_1)}},
\end{aligned}$$

and therefore $g(x,\cdot) \in L^1(\mathbb{R}^d,\mathcal{H}_2)$ uniformly in x. Inserted into (A.4) this proves that $\widehat{A}\,\psi(x)$ is uniformly bounded in $\mathcal{H}_2$. It follows from

$$\begin{aligned}
&x^\alpha\partial_x^\beta\widehat{A}\psi(x) = \int_{\mathbb{R}^{2d}} \mathrm{d}\xi\,\mathrm{d}u\,\frac{x^\alpha\mathrm{e}^{-\mathrm{i}\xi\cdot u/\varepsilon}}{\langle\xi\rangle^{2M}}\,(1+L_u)^M\partial_x^\beta\,\big[A\big(x+\tfrac{1}{2}u,\xi\big)\,\psi(u+x)\big] \\
&= \int_{\mathbb{R}^{2d}} \mathrm{d}\xi\,\mathrm{d}u\,\frac{(x+u-\mathrm{i}\varepsilon\partial_\xi)^\alpha\mathrm{e}^{-\mathrm{i}\xi\cdot u/\varepsilon}}{\langle\xi\rangle^{2M}}\,(1+L_u)^M\partial_x^\beta\,\big[A\big(x+\tfrac{1}{2}u,\xi\big)\,\psi(u+x)\big] \\
&= (-1)^{|\alpha|}\int_{\mathbb{R}^{2d}} \mathrm{d}\xi\,\mathrm{d}u\,\mathrm{e}^{-\mathrm{i}\xi\cdot u/\varepsilon}\times \\
&\qquad (x+u-\mathrm{i}\varepsilon\partial_\xi)^\alpha\,\frac{(1+L_u)^M}{\langle\xi\rangle^{2M}}\partial_x^\beta\,\big[A\big(x+\tfrac{1}{2}u,\xi\big)\,\psi(u+x)\big]
\end{aligned}$$

that one can bound $\|x^\alpha \partial_x^\beta \widehat{A}\psi(x)\|_{\mathcal{H}_2}$ for arbitrary $\alpha, \beta \in \mathbb{N}^d$ in a similar fashion, which shows that $\widehat{A}\,\psi \in \mathcal{S}(\mathbb{R}^d, \mathcal{H}_2)$. Finally the continuity of the embedding $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_1) \hookrightarrow L^1(\mathbb{R}^d, \mathcal{H}_1)$ implies the continuity of $\widehat{A} : \mathcal{S}(\mathbb{R}^d, \mathcal{H}_1) \to \mathcal{S}(\mathbb{R}^d, \mathcal{H}_2)$. □

As for scalar-valued symbols one can extend the continuous mapping $\widehat{A} : \mathcal{S}(\mathbb{R}^d, \mathcal{H}_1) \to \mathcal{S}(\mathbb{R}^d, \mathcal{H}_2)$ by duality to a continuous mapping $\widehat{A} : \mathcal{S}'(\mathbb{R}^d, \mathcal{H}_1) \to \mathcal{S}'(\mathbb{R}^d, \mathcal{H}_2)$. Since the most natural inclusion $\mathcal{S}(\mathbb{R}^d, \mathcal{H}) \hookrightarrow \mathcal{S}'(\mathbb{R}^d, \mathcal{H})$ is the anti-linear one, i.e.

$$\mathcal{S}(\mathbb{R}^d, \mathcal{H}) \ni \psi \mapsto T_\psi \in \mathcal{S}'(\mathbb{R}^d, \mathcal{H}) \quad \text{with} \quad T_\psi(\varphi) = \int_{\mathbb{R}^d} \mathrm{d}x \, \langle \psi(x), \varphi(x) \rangle_{\mathcal{H}} \,,$$

we define for $T \in \mathcal{S}'(\mathbb{R}^d, \mathcal{H}_1)$ and $\varphi \in \mathcal{S}(\mathbb{R}^d, \mathcal{H}_2)$

$$(\widehat{A}T)(\varphi) = T(\widehat{A^*}\varphi) \,.$$

This poses no problem, since $A \in S^m_\rho(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ (resp. $A \in S^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$) clearly implies that $A^* \in S^m_\rho(\mathcal{L}(\mathcal{H}_2, \mathcal{H}_1))$ (resp. $A^* \in S^w(\mathcal{L}(\mathcal{H}_2, \mathcal{H}_1))$), where A^* denotes the pointwise adjoint. Hence for $A \in S^m_\rho(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ or $A \in S^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$, $\widehat{A}$ extends to a continuous mapping

$$\widehat{A} : \mathcal{S}'(\mathbb{R}^d, \mathcal{H}_1) \to \mathcal{S}'(\mathbb{R}^d, \mathcal{H}_2) \,.$$

One introduces a special notation for such classes of operators, called pseudodifferential operators,

$$OPS^m_\rho := \left\{ \mathcal{W}_\varepsilon(A) : \, A \in S^m_\rho(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)) \right\} \,.$$

or

$$OPS^w := \left\{ \mathcal{W}_\varepsilon(A) : \, A \in S^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)) \right\} \,.$$

In the following we will sometimes denote $S^m_\rho(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ simply as S^m_ρ when no confusion about the Hilbert spaces can arise. We will also use the shorthand $S^m := S^m_0$. Notice that $S^m_\rho \subseteq S^m_{\rho'}$ for any $\rho \geq \rho'$.

Definition A.5. *For some Banach space $\mathcal{E}$ denote by $C^k_{\mathrm{b}}(\mathbb{R}^d, \mathcal{E})$ the space of $\mathcal{E}$-valued, k times continuously differentiable functions on $\mathbb{R}^d$, such that all the derivatives up to the order k are bounded. Equipped with the norm*

$$\|A\|_{C^k_{\mathrm{b}}} := \sup_{|\alpha| \leq k} \sup_{x \in \mathbb{R}^d} \|(\partial_x^\alpha A)(x)\|_{\mathcal{E}}$$

it is a Banach space.

If A belongs to $S^0(\mathcal{L}(\mathcal{H})) = S^{w=1}(\mathcal{L}(\mathcal{H}))$ then the corresponding Weyl quantization is a *bounded* operator on $L^2(\mathbb{R}^d, \mathcal{H})$. The following proposition sharpens this statement.

Proposition A.6 (Calderon-Vaillancourt). *There exists a constant* $C_{\mathrm{d}} < \infty$ *such that for every* $A \in C_{\mathrm{b}}^{2d+1}(\mathbb{R}^{2d}, \mathcal{L}(\mathcal{H}))$ *one has*

$$\left\|\widehat{A}\right\|_{\mathcal{L}(L^2(\mathbb{R}^d,\mathcal{H}))} \leq C_d \left\|A\right\|_{C_{\mathrm{b}}^{2d+1}} .$$

For the proof see Theorem 2.73 in [Fo] or Theorem 2.8.1 in [Ma$_1$], where the latter one can be translated line by line to the operator valued case.

The Calderon-Vaillancourt theorem implies, in particular, that the Weyl quantization, regarded as a map $\mathcal{W}_\varepsilon : S^0(\mathcal{L}(\mathcal{H})) \to \mathcal{L}(L^2(\mathbb{R}^d, \mathcal{H}))$, is continuous with respect to the Fréchet topology on $S^0(\mathcal{L}(\mathcal{H}))$.

Remark A.7. One of the advantages of Weyl quantization is that for $A \in S_0^0(\mathbb{R}^d, \mathcal{L}(\mathcal{H}))$ the adjoint of $\widehat{A}$ as an operator in $\mathcal{L}(L^2(\mathbb{R}^d, \mathcal{H}))$, denoted by $\widehat{A}^*$, agrees with the operator obtained as the quantization of the pointwise adjoint $\widehat{A^*}$. This can be checked by direct computation on the dense subset $\mathcal{S}(\mathbb{R}^d, \mathcal{H})$. ♢

If a symbol takes values in the bounded self-adjoint operators, then its quantization is expected to be self-adjoint too on a suitable domain. It is easy to see that if $A \in S_0^0(\mathbb{R}^d, \mathcal{L}_{\mathrm{sa}}(\mathcal{H}))$, then $\widehat{A} \in \mathcal{L}_{\mathrm{sa}}(L^2(\mathbb{R}^d, \mathcal{H}))$. However, if $\widehat{A}$ is unbounded the question of self-adjointness becomes more subtle. We close this section with a result concerning essential self-adjointness of operators which are obtained through Weyl-quantization. The following result is taken from [DiSj], Proposition 8.5.

Proposition A.8. *Let* $A \in S^w(\mathcal{L}(\mathcal{H}))$ *such that* $A + \mathrm{i}$ *is elliptic in the sense that* $\|A(q,p) + \mathrm{i}\| \geq C w(q,p)$ *for some constant* $C > 0$. *Then* $\widehat{A}$ *is essentially self-adjoint on* $\mathcal{S}(\mathbb{R}^d, \mathcal{H})$ *for* ε *sufficiently small.*

A.2 Composition of symbols: the Weyl-Moyal product

The behavior of the symbol classes with respect to the pointwise product is very simple, as can be checked by using the Leibniz rule.

Proposition A.9. (i) *If* $A \in S_\rho^{m_1}(\mathcal{L}(\mathcal{H}_2, \mathcal{H}_3))$ *and* $B \in S_\rho^{m_2}(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$, *then* AB *belongs to* $S_\rho^{m_1+m_2}(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_3))$ *for every* $m_1, m_2 \in \mathbb{R}$.

(ii) *If* $A \in S^{w_1}(\mathcal{L}(\mathcal{H}_2, \mathcal{H}_3))$ *and* $B \in S^{w_2}(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$, *then* AB *belongs to* $S^{w_1 w_2}(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_3))$ *for arbitrary order functions* w_1, w_2.

The crucial observation which makes the pseudodifferential calculus so useful is that one can define an associative product in the space of classical symbols which corresponds to the composition of the operators. Given $A \in S_\rho^{m_1}(\mathcal{L}(\mathcal{H}_2, \mathcal{H}_3))$ and $B \in S_\rho^{m_2}(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$, then we know that $\widehat{A}\,\widehat{B}$ maps $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_1)$ into $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_3)$. As in the case of scalar symbols this map is again a pseudodifferential operator, cf. Theorem 2.47 in [Fo] and Proposition 13.9 in [DiSj].

Proposition A.10. *Let $A \in S^{m_1}_\rho(\mathcal{L}(\mathcal{H}_2,\mathcal{H}_3))$ and $B \in S^{m_2}_\rho(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$, then $\widehat{A}\widehat{B} = \widehat{C}$, with $C \in S^{m_1+m_2}_\rho(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_3))$ given through*

$$C(q,p) = \exp\left(\frac{\mathrm{i}\,\varepsilon}{2}\left(\nabla_p\cdot\nabla_x - \nabla_\xi\cdot\nabla_q\right)\right) A(q,p)B(x,\xi)\Big|_{x=q,\xi=p} =: A\,\widetilde{\sharp}\,B\,. \tag{A.7}$$

Note that it is part of the statement of Proposition A.10 that (A.7) really defines a symbol in $S^{m_1+m_2}_\rho(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_3))$, since a priori the expression (A.7) is only well defined as an operator of convolution with the exponential e.g. for A, B with compact support. The analogous statement holds true for the classes S^w.

Proposition A.11. *Let $A \in S^{w_1}(\mathcal{L}(\mathcal{H}_2,\mathcal{H}_3))$ and $B \in S^{w_2}(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$, then $\widehat{A}\widehat{B} = \widehat{C}$, with $C \in S^{w_1 w_2}(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_3))$ given through (A.7).*

The symbol $A\,\widetilde{\sharp}\,B$ is called the **Weyl product** (or the twisted product) of the symbols A and B. Note that $S^0_\rho(\mathcal{L}(\mathcal{H}))$ and $S^\infty_\rho(\mathcal{L}(\mathcal{H})) := \bigcup_{m\in\mathbb{R}} S^m_\rho(\mathcal{L}(\mathcal{H}))$ are algebras with respect to the Weyl product $\widetilde{\sharp}$.

Since the product $A\,\widetilde{\sharp}\,B$ depends on ε by construction, one can expand the Weyl product in orders of ε. To this end, it is convenient to define suitable classes of ε-dependent symbols, called **semiclassical symbols**, which – roughly speaking – are close to a power series in ε of classical symbols with nicer and nicer behavior at infinity. Our definition is a special case of the standard ones (see [Fo, Hö$_2$]).

Definition A.12. *A map $A : [0,\varepsilon_0) \to S^m_\rho(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)), \varepsilon \mapsto A_\varepsilon$ is a semiclassical symbol of order m and weight ρ if there exists a sequence $\{A_j\}_{j\in\mathbb{N}}$ with $A_j \in S^{m-j\rho}_\rho(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$ such that for every $n \in \mathbb{N}$ one has that*

$$\varepsilon^{-n}\left(A_\varepsilon - \sum_{j=0}^{n-1}\varepsilon^j A_j\right) \in S^{m-n\rho}_\rho(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$$

uniformly *in ε, in the following sense: For any $k \in \mathbb{N}$ there exists a constant $C_{n,k}$ such that for any $\varepsilon \in [0,\varepsilon_0)$ one has*

$$\Big\|A_\varepsilon - \sum_{j=0}^{n-1}\varepsilon^j A_j\Big\|_k^{(m-n\rho)} \le C_{n,k}\,\varepsilon^n\,, \tag{A.8}$$

where $\|\cdot\|_k^{(m)}$ is the k^{th} Fréchet semi-norm in $S^m_\rho(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$, introduced in (A.5).

The space of semiclassical symbols of order m and weight ρ is denoted as $S^m_\rho(\varepsilon,\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$ or, if clear from the context or if no specification is required, as $S^m_\rho(\varepsilon)$.

A_0 is called the **principal symbol** and A_1 is called the **subprincipal symbol** of A_ε. If condition (A.8) is fulfilled, one writes

$$A_\varepsilon \asymp \sum_{j\geq 0} \varepsilon^j A_j \quad \text{in } S^m_\rho(\varepsilon)$$

and one says that A_ε is asymptotically equivalent to the series $\sum_{j\geq 0} \varepsilon^j A_j$ in $S^m_\rho(\varepsilon)$. If A_ε is asymptotically equivalent to the series in which $A_j = 0$ for every $j \in \mathbb{N}$, we write $A_\varepsilon = \mathcal{O}(\varepsilon^\infty)$. To be precise, we should write $A_\varepsilon = \mathcal{O}(\varepsilon^\infty)$ in $S^m_\rho(\varepsilon)$, but the latter specification is omitted whenever it is unambiguous from the context.

Again the previous definitions and all the following translate unambiguously to the symbols defined through order functions with the only difference that the coefficients in an asymptotic expansion of $A_\varepsilon \in S^w(\varepsilon)$ are all in the same space S^w.

Remark A.13. Notice that for $A_\varepsilon \in S^0_0(\varepsilon, \mathcal{L}(\mathcal{H}))$ the Calderon-Vaillancourt theorem, Proposition A.6, gives immediately that

$$\sup_{\varepsilon\in[0,\varepsilon_0)} \left\|\widehat{A}_\varepsilon\right\|_{\mathcal{L}(L^2(\mathbb{R}^d,\mathcal{H}))} \leq C < \infty\,,$$

since all the semi-norms appearing in $\|A_\varepsilon\|_{C^{2d+1}_{\mathrm{b}}}$ are bounded uniformly by definition of $S^0_0(\varepsilon, \mathcal{L}(\mathcal{H}))$. ♢

In general a formal power series $\sum_{j\geq 0} \varepsilon^j A_j$ is not convergent, but it is always the asymptotic expansion of a (non unique) semiclassical symbol A_ε. This is because one can obtain a semiclassical symbol from a formal power series through

$$A_\varepsilon = \sum_{j=0}^{N(\varepsilon)} \varepsilon^j A_j\,,$$

with $N(\varepsilon) \to \infty$ as $\varepsilon \to 0$ chosen in such a way that the semi-norms $\|A_\varepsilon\|^{(m)}_k$ remain uniformly bounded for $\varepsilon \in (0, \varepsilon_0]$. For an explicit construction of $N(\varepsilon)$ see e.g. Proposition 2.26 in [Fo].

Proposition A.14. *Let be $\{A_j\}_{j\in\mathbb{N}}$ an arbitrary sequence such that $A_j \in S^{m-j\rho}_\rho$. Then there exists $A_\varepsilon \in S^m_\rho(\varepsilon)$ such that $A_\varepsilon \asymp \sum_{j\geq 0} \varepsilon^j A_j$ in $S^m_\rho(\varepsilon)$ and A_ε is unique up to $\mathcal{O}(\varepsilon^\infty)$, in the sense that the difference of two such symbols is $\mathcal{O}(\varepsilon^\infty)$ in $S^m_\rho(\varepsilon)$. The semiclassical symbol A_ε is called a* **resummation** *of the formal symbol $\sum_{j\geq 0} \varepsilon^j A_j$.*

The Weyl product of two semiclassical symbols is again a semiclassical symbol with an explicit asymptotic expansion. For the proof in the scalar case see Theorem 2.49 in [Fo], which can be adapted to the operator valued case with minor changes.

Proposition A.15 (Product rule). *If*

$$A_\varepsilon \asymp \sum_{j\geq 0} \varepsilon^j A_j \qquad \text{in } S^{m_1}_\rho(\varepsilon, \mathcal{L}(\mathcal{H}_3, \mathcal{H}_2))$$

and

$$B_\varepsilon \asymp \sum_{j\geq 0} \varepsilon^j B_j \qquad \text{in } S^{m_2}_\rho(\varepsilon, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))\,,$$

then $A_\varepsilon \mathbin{\widetilde{\sharp}} B_\varepsilon \in S^{m_1+m_2}_\rho(\varepsilon, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_3))$ *has an asymptotic expansion given by*

$$\left(A_\varepsilon \mathbin{\widetilde{\sharp}} B_\varepsilon\right)_k (q,p) = (2\mathrm{i})^{-k} \sum_{|\alpha|+|\beta|+j+l=k} \frac{(-1)^{|\alpha|}}{|\alpha|!|\beta|!} \left((\partial_q^\alpha \partial_p^\beta A_j)(\partial_p^\alpha \partial_q^\beta B_l)\right)(q,p) \tag{A.9}$$

where it is understood that $k, j, l \in \mathbb{N}$ *and* $\alpha, \beta \in \mathbb{N}^d$.

Most important for our implicit calculations are the leading orders:

$$(A_\varepsilon \mathbin{\widetilde{\sharp}} B_\varepsilon)_0 = A_0 B_0$$

and

$$(A_\varepsilon \mathbin{\widetilde{\sharp}} B_\varepsilon)_1 = A_0 B_1 + A_1 B_0 - \frac{\mathrm{i}}{2}\{A_0, B_0\}\,,$$

where $\{\cdot,\cdot\}$ denotes the Poisson bracket defined through

$$\{A, B\} = \sum_{j=1}^{d} \frac{\partial A}{\partial p_j}\frac{\partial B}{\partial q_j} - \frac{\partial A}{\partial q_j}\frac{\partial B}{\partial p_j}\,. \tag{A.10}$$

Notice that even for $A, B \in S^m_\rho(\mathcal{L}(\mathcal{H}))$, in general, $\{A, B\} \neq -\{B, A\}$ since operator-valued derivatives do not commute, in particular $\{A, A\} \neq 0$. The usual Poisson algebra is recovered in the special case in which one of the two arguments is a multiple of the identity, i.e. $A(z) = a(z)\mathbf{1}_\mathcal{H}$. Then a very useful formula for the commutator follows,

$$\left[\, a_\varepsilon,\, B_\varepsilon \,\right]_{\widetilde{\sharp}} := a_\varepsilon \mathbin{\widetilde{\sharp}} B_\varepsilon - B_\varepsilon \mathbin{\widetilde{\sharp}} a_\varepsilon \asymp -\mathrm{i}\,\varepsilon\,\{\, a_\varepsilon,\, B_\varepsilon \,\} + \mathcal{O}(\varepsilon^3)\,. \tag{A.11}$$

It is convenient to introduce also the space of the formal power series with coefficients in $S^\infty_\rho(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$. Denote by $M^m_\rho(\varepsilon, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ the subspace of the formal power series with a resummation in $S^m_\rho(\varepsilon, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$, i.e.

$$M^m_\rho(\varepsilon, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)) := \left\{ \sum_{j\geq 0} \varepsilon^j A_j : A_j \in S^{m-j\rho}_\rho(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)) \right\}.$$

In the context of formal power series, the product defined by (A.9) is called the **Moyal product** and denoted simply as $\sharp$. Notice that $\sharp$ defines a map from

$$M^{m_1}_\rho(\varepsilon,\mathcal{L}(\mathcal{H}_2,\mathcal{H}_3))\times M^{m_2}_\rho(\varepsilon,\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)) \quad \text{to} \quad M^{m_1+m_2}_\rho(\varepsilon,\mathcal{L}(\mathcal{H}_1,\mathcal{H}_3))\,.$$

The Moyal product can also be regarded as a map from $M^{m_1}_\rho(\varepsilon,\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))\times M^{m_2}_\rho(\varepsilon,\mathcal{H}_1)$ to $M^{m_1+m_2}_\rho(\varepsilon,\mathcal{H}_2)$, where in (A.9) the operator A and its derivatives act on the vector B and its derivatives.

To sum up the previous discussion, we stress that one can prove statements on three levels: formal symbols (i.e. formal power series), semiclassical symbols, and operators from $\mathcal{S}(\mathbb{R}^d,\mathcal{H}_1)\subseteq L^2(\mathbb{R}^d,\mathcal{H}_1)$ to $\mathcal{S}(\mathbb{R}^d,\mathcal{H}_2)\subseteq L^2(\mathbb{R}^d,\mathcal{H}_2)$. A simple example illustrates the interplay between these levels. Suppose that two formal symbols $A\in M^{m_1}_\rho(\varepsilon,\mathcal{L}(\mathcal{H}))$ and $B\in M^{m_2}_\rho(\varepsilon,\mathcal{L}(\mathcal{H}))$ Moyal commute, i.e. $[A,B]_\sharp = A\sharp B - B\sharp A = 0$. Let $A_\varepsilon\in S^{m_1}_\rho(\varepsilon,\mathcal{L}(\mathcal{H}))$ and $B_\varepsilon\in S^{m_2}_\rho(\varepsilon,\mathcal{L}(\mathcal{H}))$ be any two resummations of A respectively B. Since we know *a priori* from Proposition A.15 that the Weyl product $A_\varepsilon\,\widetilde{\sharp}\,B_\varepsilon$ belongs to $S^{m_1+m_2}_\rho(\varepsilon,\mathcal{L}(\mathcal{H}))$, it follows that the Weyl commutator $[A_\varepsilon,B_\varepsilon]_{\widetilde{\sharp}}$ is asymptotically close to zero in $S^{m_1+m_2}_\rho(\varepsilon,\mathcal{L}(\mathcal{H}))$, which can be rephrased in the following way: for any $n,k\in\mathbb{N}$ there exists a constant $C_{n,k}$ such that for any $\varepsilon\in[0,\varepsilon_0)$ one has

$$\left\|\,[A_\varepsilon,B_\varepsilon]_{\widetilde{\sharp}}\,\right\|_k^{(m_1+m_2-n\rho)}\leq C_{n,k}\;\varepsilon^n\,.$$

If $\rho>0$ we obtain that definitely $m_1+m_2-n\rho\leq 0$ for some $n\in\mathbb{N}$ and then Proposition A.6 assures that the operator commutator $[\widehat{A}_\varepsilon,\widehat{B}_\varepsilon]$ can be bounded in the $\mathcal{L}(L^2(\mathbb{R}^d,\mathcal{H}))$-norm. Moreover, for $\rho>0$, we can conclude that $[\widehat{A}_\varepsilon,\widehat{B}_\varepsilon]$ is a smoothing operator (i.e. it belongs to $OPS^{-\infty}_\rho := \cap_{m\in\mathbb{R}}OPS^m_\rho$) and in particular one can prove that it is a "small" bounded operator between the Sobolev spaces $H^q(\mathbb{R}^d,\mathcal{H})$ and $H^{q+r}(\mathbb{R}^d,\mathcal{H})$ for any $q,r\in\mathbb{N}$. To be precise, for any $q,r,n\in\mathbb{N}$ there exist a constant $C_{n,q,r}$ such that

$$\left\|\left[\widehat{A}_\varepsilon,\widehat{B}_\varepsilon\right]\right\|_{\mathcal{L}(H^q,H^{q+r})}\leq C_{n,q,r}\,\varepsilon^n$$

for any $\varepsilon\in[0,\varepsilon_0)$, where H^q stands for $H^q(\mathbb{R}^d,\mathcal{H})$.

On the other hand, notice that for $\rho=0$ and $m_1+m_2=:m>0$ it is not possible to conclude from $[A,B]_\sharp=0$ that $[\widehat{A}_\varepsilon,\widehat{B}_\varepsilon]$ is a bounded operator, since it could happen – for example – that $[A_\varepsilon,B_\varepsilon]_{\widetilde{\sharp}} = \mathrm{e}^{-1/\varepsilon}\langle p\rangle^m$, which is asymptotically close to zero in $S^m_\rho(\varepsilon)$. The same problem occurs when working with semiclassical symbols in $S^w(\varepsilon)$.

Hence we introduce the following synthetic notation.

Definition A.16. *Let be A_ε and B_ε semiclassical symbols in $S^m_\rho(\varepsilon)$. We say that $B_\varepsilon = A_\varepsilon+\mathcal{O}_{-\infty}(\varepsilon^\infty)$ if $B_\varepsilon - A_\varepsilon$ is asymptotically close to zero in $S^m_\rho(\varepsilon)$ for $\rho>0$.*

With a little abuse, we employ the same notation for pseudodifferential operators too, i.e. we write $\widehat{B}_\varepsilon=\widehat{A}_\varepsilon+\mathcal{O}_{-\infty}(\varepsilon^\infty)$ if $B_\varepsilon=A_\varepsilon+\mathcal{O}_{-\infty}(\varepsilon^\infty)$.

As noticed above this is a strong concept of closeness, since it implies that $\widehat{B}_\varepsilon - \widehat{A}_\varepsilon$ is a smoothing operator. Compare with the following weaker concept.

Definition A.17. *Let be R_ε and S_ε two ε-dependent operators on $\mathcal{H}$. We say that $R_\varepsilon = S_\varepsilon + \mathcal{O}_0(\varepsilon^\infty)$ if for every $n \in \mathbb{N}$ there exists a constant C_n such that*

$$\|R_\varepsilon - S_\varepsilon\|_{\mathcal{L}(L^2(\mathbb{R}^d,\mathcal{H}_1),L^2(\mathbb{R}^d,\mathcal{H}_2))} \leq C_n \varepsilon^n$$

for every $\varepsilon \in [0, \varepsilon_0)$. In such a case we say that R_ε is $\mathcal{O}_0(\varepsilon^\infty)$-close to S_ε.

The notation A_ε for a semiclassical symbol was introduced only for sake of clear presentation in the present section. In the main body of the monograph, we use the same symbol A for an element in $S^m_\rho(\varepsilon)$ and its expansion in $M^m_\rho(\varepsilon)$. In particular, we drop the subscript ε from A_ε.

B Operator-valued Weyl calculus for τ-equivariant symbols

The pseudodifferential calculus for scalar-valued symbols defined on the phase space $T^*\mathbb{R}^d = \mathbb{R}^{2d}$ can be translated to the phase space $T^*\mathbb{T}^d = \mathbb{T}^d \times \mathbb{R}^d$, $\mathbb{T}^d$ a flat torus, by restricting to periodic functions and symbols. This approach is used by Gérard and Nier [GeNi] in the context of scattering theory in periodic media.

In this appendix we present a similar approach to Weyl quantization of operator-valued symbols which are not exactly periodic, but τ-equivariant with respect to some nontrivial representation τ of the group of lattice translations. We obtain a pseudodifferential and semiclassical calculus which can be applied to τ-equivariant symbols like the Schrödinger Hamiltonian with periodic potential in Bloch-Floquet representation of Chapter 5. In particular, the full computational power of the usual Weyl calculus is retained. The strategy is to use the strong results available for phase space $\mathbb{R}^{2d}$ by restricting to functions which are τ-equivariant in the configurational variable.

Let $\Gamma \subset \mathbb{R}^d$ be a regular lattice generated through the basis $\{\gamma_1, \ldots, \gamma_d\}$, $\gamma_j \in \mathbb{R}^d$, i.e.

$$\Gamma = \left\{ x \in \mathbb{R}^d : x = \sum_{j=1}^{d} \alpha_j \, \gamma_j \ \text{ for some } \alpha \in \mathbb{Z}^d \right\} .$$

Clearly the translations on $\mathbb{R}^d$ by elements of Γ form an abelian group isomorphic to $\mathbb{Z}^d$. The centered fundamental cell of Γ is denoted as

$$M = \left\{ x \in \mathbb{R}^d : x = \sum_{j=1}^{d} \alpha_j \, \gamma_j \ \text{ for } \alpha_j \in [-\tfrac{1}{2}, \tfrac{1}{2}] \right\} .$$

Let $\mathcal{H}$ be a separable Hilbert space and let τ be a representation of Γ in $\mathcal{L}^*(\mathcal{H})$, the group of invertible elements of $\mathcal{L}(\mathcal{H})$, i.e. a group homomorphism

$$\tau : \Gamma \to \mathcal{L}^*(\mathcal{H}), \qquad \gamma \mapsto \tau(\gamma) \, .$$

If more than one Hilbert space appears, then τ denotes a collection of such representations, i.e. one on each Hilbert space.

Warning: In the application of the results of this appendix to Bloch electrons in Chapter 5 the lattice Γ corresponds to the dual lattice Γ^* in momentum space $\mathbb{R}^d$.

Let L_γ be the operator of translation by $\gamma \in \Gamma$ on $\mathcal{S}(\mathbb{R}^d, \mathcal{H})$, i.e. $(L_\gamma \varphi)(x) = \varphi(x - \gamma)$, and extend it by duality to distributions, i.e. for $T \in \mathcal{S}'(\mathbb{R}^d, \mathcal{H})$ let $(L_\gamma T)(\varphi) = T(L_{-\gamma}\varphi)$.

Definition B.1. *A tempered distribution $T \in \mathcal{S}'(\mathbb{R}^d, \mathcal{H})$ is said to be* τ-equivariant *if*

$$L_\gamma T = \tau(\gamma) T \quad \textit{for all } \gamma \in \Gamma\,,$$

where $\big(\tau(\gamma)T\big)(\varphi) = T\big(\tau(\gamma)^{-1}\varphi\big)$ for $\varphi \in \mathcal{S}(\mathbb{R}^d, \mathcal{H})$. The subspace of τ-equivariant distributions is denoted as $\mathcal{S}'_\tau$. Analogously we define

$$\mathcal{H}_\tau = \Big\{ \psi \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathcal{H}) : \psi(x - \gamma) = \tau(\gamma)\, \psi(x) \quad \textit{for all } \gamma \in \Gamma \Big\}\,,$$

which, equipped with the inner product

$$\langle \varphi, \psi \rangle_{\mathcal{H}_\tau} = \int_M \mathrm{d}x\, \langle \varphi(x), \psi(x) \rangle_{\mathcal{H}}\,,$$

is a Hilbert space. Clearly

$$C^\infty_\tau = \Big\{ \psi \in C^\infty(\mathbb{R}^d, \mathcal{H}) : \psi(x - \gamma) = \tau(\gamma)\, \psi(x) \quad \textit{for all } \gamma \in \Gamma \Big\}\,,$$

is a dense subspace of $\mathcal{H}_\tau$.

Notice that if τ is a unitary representation, then for any $\varphi, \psi \in \mathcal{H}_\tau$ the map $x \mapsto \langle \varphi(x), \psi(x) \rangle_{\mathcal{H}}$ is periodic, since

$$\langle \varphi(x - \gamma), \psi(x - \gamma) \rangle_{\mathcal{H}} = \langle \tau(\gamma)\varphi(x), \tau(\gamma)\psi(x) \rangle_{\mathcal{H}} = \langle \varphi(x), \psi(x) \rangle_{\mathcal{H}}\,.$$

Now that we have τ-equivariant functions, we define τ-equivariant symbols.

Definition B.2. *A symbol $A_\varepsilon \in S^w(\varepsilon, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ is* τ-equivariant *(more precisely (τ_1, τ_2)-equivariant), if*

$$A_\varepsilon(q - \gamma, p) = \tau_2(\gamma)\, A_\varepsilon(q, p)\, \tau_1(\gamma)^{-1} \quad \textit{for all } \gamma \in \Gamma\,.$$

The space of τ-equivariant symbols is denoted as $S^w_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$.

Notice that the coefficients in the asymptotic expansion of a τ-equivariant semiclassical symbol must be as well τ-equivariant, i.e. if $A_\varepsilon \asymp \sum_{j=0}^\infty \varepsilon^j A_j$, $A_\varepsilon \in S^w_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$, then $A_j \in S^w_\tau(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$.

Given any τ-equivariant symbol $A \in S^w_\tau(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$, one can consider the usual Weyl quantization $\widehat{A}$, regarded as an operator acting on $\mathcal{S}'(\mathbb{R}^d, \mathcal{H}_1)$ with distributional integral kernel

$$K_A(x,y) = \frac{1}{(2\pi\varepsilon)^d} \int_{\mathbb{R}^d} \mathrm{d}\xi \, A\big(\tfrac{1}{2}(x+y),\xi\big) \, \mathrm{e}^{\mathrm{i}\xi\cdot(x-y)/\varepsilon} \,. \tag{B.1}$$

Notice that integral kernel associated to a τ-equivariant symbol A is τ-equivariant in the following sense:

$$K_A(x-\gamma, y-\gamma) = \tau_2(\gamma)\, K_A(x,y)\, \tau_1(\gamma)^{-1} \quad \text{for all } \gamma \in \Gamma \,. \tag{B.2}$$

The simple but important observation is that the space of τ-equivariant distributions is invariant under the action of quantizations of τ-equivariant symbols.

Proposition B.3. *Let $A \in S^w_\tau(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$, then*

$$\widehat{A}\, \mathcal{S}'_{\tau_1}(\mathbb{R}^d,\mathcal{H}_1) \subset \mathcal{S}'_{\tau_2}(\mathbb{R}^d,\mathcal{H}_2) \,.$$

Proof. Since $\widehat{A}$ maps $\mathcal{S}'(\mathbb{R}^d,\mathcal{H}_1)$ continuously into $\mathcal{S}'(\mathbb{R}^d,\mathcal{H}_2)$, we only need to show that $(L_\gamma \widehat{A} T)(\varphi) = (\tau_2(\gamma)\widehat{A}T)(\varphi)$ for all $T \in \mathcal{S}'_{\tau_1}(\mathbb{R}^d,\mathcal{H}_1)$ and $\varphi \in \mathcal{S}(\mathbb{R}^d,\mathcal{H}_2)$.

To this end notice that as acting on $\mathcal{S}(\mathbb{R}^d,\mathcal{H}_2)$ one finds by direct computation using (B.1) that $\widehat{A^*}\, L_\gamma = L_\gamma\, (\tau_1(\gamma)^{-1})^*\, \widehat{A^*}\, \tau_2(\gamma)^*$. Indeed, let $\psi \in \mathcal{S}(\mathbb{R}^d,\mathcal{H}_2)$, then

$$\begin{aligned}
\big(\widehat{A^*}\, L_\gamma\, \psi\big)(x) &= \int_{\mathbb{R}^d} \mathrm{d}y\, K_{A^*}(x,y)\, \psi(y-\gamma) = \int_{\mathbb{R}^d} \mathrm{d}y\, K_{A^*}(x,y+\gamma)\, \psi(y) \\
&= \int_{\mathbb{R}^d} \mathrm{d}y\, (\tau_1(\gamma)^{-1})^*\, K_{A^*}(x-\gamma,y)\, \tau_2(\gamma)^*\, \psi(y) \\
&= \Big(L_\gamma\, (\tau_1(\gamma)^{-1})^*\, \widehat{A^*}\, \tau_2(\gamma)^*\, \psi\Big)(x)
\end{aligned}$$

Hence, using the fact that τ is a representation and that $L_\gamma T = \tau_1(\gamma) T$,

$$\begin{aligned}
(L_\gamma \widehat{A} T)(\varphi) &= T(\widehat{A}^*\, L_{-\gamma}\, \varphi) = T(L_{-\gamma}\, \tau_1(\gamma)^*\, \widehat{A}^*\, (\tau_2(\gamma)^{-1})^*\, \varphi) \\
&= (\tau_2(\gamma)\, \widehat{A}\, \tau_1(\gamma)^{-1}\, L_\gamma\, T)(\varphi) = (\tau_2(\gamma)\, \widehat{A}\, T)(\varphi) \,.
\end{aligned}$$

□

Next observe that τ-equivariance of symbols is preserved under the pointwise product, the Weyl product and the Moyal product.

Proposition B.4. *Let $A_\varepsilon \in S^{w_1}_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_2,\mathcal{H}_3))$ and $B_\varepsilon \in S^{w_2}_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$, then $A_\varepsilon B_\varepsilon \in S^{w_1 w_2}_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_1,\mathcal{H}_3))$ and $A_\varepsilon \mathbin{\widetilde{\sharp}} B_\varepsilon \in S^{w_1 w_2}_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_1,\mathcal{H}_3))$.*

Proof. One has

$$\begin{aligned}
A_\varepsilon(q-\gamma,p) B_\varepsilon(q-\gamma,p) &= \tau_3(\gamma) A_\varepsilon(q,p) \tau_2(\gamma)^{-1} \tau_2(\gamma) B_\varepsilon(q,p) \tau_1(\gamma)^{-1} \\
&= \tau_3(\gamma) A_\varepsilon(q,p) B_\varepsilon(q,p) \tau_1(\gamma)^{-1} \,,
\end{aligned}$$

which shows $A_\varepsilon B_\varepsilon \in S^{w_1 w_2}_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_1,\mathcal{H}_3))$ and inserted into (A.7) yields immediately also $A_\varepsilon \mathbin{\widetilde{\sharp}} B_\varepsilon \in S^{w_1 w_2}_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_1,\mathcal{H}_3))$. □

As for the Moyal product of formal symbol, an analogous statement holds true.

A not completely obvious fact is the following variant of the Calderon-Vaillancourt theorem.

Theorem B.5. *Let $A \in S^{w=1}_{\tau}(\mathcal{L}(\mathcal{H}))$ and τ_1, τ_2 unitary representations of Γ in $\mathcal{L}(\mathcal{H})$, then $\widehat{A} \in \mathcal{L}(\mathcal{H}_{\tau_1}, \mathcal{H}_{\tau_2})$ and for $A_\varepsilon \in S^{w=1}_{\tau}(\varepsilon, \mathcal{L}(\mathcal{H}))$ we have that $\sup_{\varepsilon\in[0,\varepsilon_0)} \|\widehat{A}_\varepsilon\|_{\mathcal{L}(\mathcal{H}_{\tau_1},\mathcal{H}_{\tau_2})} < \infty$.*

Proof. Fix $n > d/2$ and let $w(x) = \langle x\rangle^{-n}$. We consider the weighted L^2-space

$$L^2_w = \left\{ \psi \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathcal{H}) : \int_{\mathbb{R}^d} \mathrm{d}x\, w(x)^2 |\psi(x)|^2 < \infty \right\}.$$

Let $j = 1, 2$, then $\mathcal{H}_{\tau_j} \subset L^2_w$ and for any $\psi \in \mathcal{H}_{\tau_j}$ one has the norm equivalence

$$C_1 \|\psi\|_{\mathcal{H}_{\tau_j}} \leq \|\psi\|_{L^2_w} \leq C_2 \|\psi\|_{\mathcal{H}_{\tau_j}} \tag{B.3}$$

for appropriate constants $0 < C_1, C_2 < \infty$. The first inequality in (B.3) is obvious and the second one follows by exploiting τ_j-equivariance of ψ and unitarity of τ_j:

$$\begin{aligned}\|\psi\|^2_{L^2_w} &= \sum_{\gamma\in\Gamma} \int_{M+\gamma} \mathrm{d}x\, w(x)^2 \, \|\tau_j(\gamma)^{-1}\psi(x)\|^2_{\mathcal{H}} = \sum_{\gamma\in\Gamma} \int_{M+\gamma} \mathrm{d}x\, w(x)^2 \, \|\psi(x)\|^2_{\mathcal{H}} \\ &\leq \sum_{\gamma\in\Gamma} \sup_{x\in M+\gamma} \left\{ w(x)^2 \right\} \int_M \mathrm{d}x\, \|\psi(x)\|^2_{\mathcal{H}} \leq C_2 \, \|\psi\|_{\mathcal{H}_{\tau_j}}.\end{aligned}$$

According to (B.3) it suffices to show that $\widehat{A} \in \mathcal{L}(L^2_w)$ and to estimate the norm of $\widehat{A}_\varepsilon$ in this space.

Let $\psi \in C^\infty_{\tau_1}(\mathbb{R}^d, \mathcal{H})$, then by the general theory $\widehat{A}\psi$ is smooth as well (cf. [Fo], Corollary 2.62) and thus, according to Proposition B.3, $\widehat{A}\psi \in C^\infty_{\tau_2}(\mathbb{R}^d, \mathcal{H})$. Hence we can use (B.3) and find

$$\left\|\widehat{A}\psi\right\|_{L^2_w} = \left\|w\widehat{A}\psi\right\|_{L^2} \leq \left\|w\widehat{A}w^{-1}\right\|_{\mathcal{L}(L^2)} \left\|w\psi\right\|_{L^2} = \left\|w\widehat{A}w^{-1}\right\|_{\mathcal{L}(L^2)} \left\|\psi\right\|_{L^2_w}.$$

However, by Proposition A.10, we have that $w \,\widetilde{\sharp}\, A \,\widetilde{\sharp}\, w^{-1} \in S^{w=1}(\varepsilon, \mathcal{L}(\mathcal{H}))$. Thus from the usual Calderon-Vaillancourt theorem it follows that

$$\left\| w \;\widehat{A}\; w^{-1} \right\|_{\mathcal{L}(L^2)} \leq C_d \left\| \, w \,\widetilde{\sharp}\, A \,\widetilde{\sharp}\, w^{-1} \right\|_{C^{2d+1}_{\mathrm{b}}(\mathbb{R}^{2d})}.$$

This shows that for $A \in S^{w=1}_{\tau}(\mathcal{L}(\mathcal{H}))$ we have $\widehat{A} \in \mathcal{L}(\mathcal{H}_{\tau_1}, \mathcal{H}_{\tau_2})$. Since also $w \,\widetilde{\sharp}\, A_\varepsilon \,\widetilde{\sharp}\, w^{-1} \in S^{w=1}(\varepsilon, \mathcal{L}(\mathcal{H}))$ for $A_\varepsilon \in S^{w=1}_{\tau}(\varepsilon, \mathcal{L}(\mathcal{H}))$, we conclude that

$$\sup_{\varepsilon\in[0,\varepsilon_0)} \|\widehat{A}_\varepsilon\|_{\mathcal{L}(\mathcal{H}_{\tau_1},\mathcal{H}_{\tau_2})} < \infty$$

by the same argument. □

Remark B.6. It is clear from the proof that the previous result still holds true under the weaker assumption that τ_1 and τ_2 are uniformly bounded, i.e. that

$$\sup_{\gamma\in\Gamma} \|\tau_j(\gamma)\|_{\mathcal{L}(\mathcal{H})} \leq C\,, \quad j = 1, 2\,.$$

♢

Finally we would also like to show that for $A \in S^w_\tau(\mathcal{L}(\mathcal{H}))$ the adjoint of $\widehat{A}$ as an operator in $\mathcal{L}(\mathcal{H}_\tau)$, denoted by $\widehat{A}^\dagger$, is given through the quantization of the pointwise adjoint, i.e. through $\widehat{A^*}$. Here it is crucial that τ is a unitary representation.

Proposition B.7. *Let $S^w_\tau(\mathcal{L}(\mathcal{H}))$ with a unitary representation τ (with $\tau_1 = \tau_2 = \tau$) and let $\widehat{A}^\dagger$ be the adjoint of $\widehat{A} \in \mathcal{L}(\mathcal{H}_\tau)$, then $\widehat{A}^\dagger = \widehat{A^*}$.*

Proof. Let $\psi \in \mathcal{H}_\tau$ and $\varphi \in C^\infty_\tau$ such that $\widetilde{\varphi} := \mathbf{1}_M\,\varphi \in C^\infty_0(\mathbb{R}^d, \mathcal{H})$, where $\mathbf{1}_M$ denotes the characteristic function of the set M. Such φ are dense in $\mathcal{H}_\tau$ and the corresponding $\widetilde{\varphi}$ can be used as a test function:

$$\begin{aligned}
\big\langle \varphi, \widehat{A}\psi\big\rangle_{\mathcal{H}_\tau} &= \int_M \mathrm{d}x\, \big\langle \varphi(x),\, (\widehat{A}\psi)(x)\big\rangle_{\mathcal{H}} = \int_{\mathbb{R}^d} \mathrm{d}x\, \big\langle \widetilde{\varphi}(x),\, (\widehat{A}\psi)(x)\big\rangle_{\mathcal{H}} \\
&= \int_{\mathbb{R}^d} \mathrm{d}x\, \big\langle (\widehat{A^*}\widetilde{\varphi})(x),\, \psi(x)\big\rangle_{\mathcal{H}} \\
&= \int_{\mathbb{R}^d} \mathrm{d}x\, \Big\langle \int_{\mathbb{R}^d} \mathrm{d}y\, K_{A^*}(x,y)\widetilde{\varphi}(y),\, \psi(x)\Big\rangle_{\mathcal{H}} \\
&= \int_{\mathbb{R}^d} \mathrm{d}x\, \Big\langle \int_M \mathrm{d}y\, K^*_A(x,y)\widetilde{\varphi}(y),\, \psi(x)\Big\rangle_{\mathcal{H}} \\
&= \int_M \mathrm{d}x \sum_{\gamma\in\Gamma} \Big\langle \int_M \mathrm{d}y\, K^*_A(x+\gamma,y)\widetilde{\varphi}(y),\, \psi(x+\gamma)\Big\rangle_{\mathcal{H}} \\
&= \int_M \mathrm{d}x \sum_{\gamma\in\Gamma} \Big\langle \int_M \mathrm{d}y\, \tau^{-1}(\gamma)K^*_A(x,y-\gamma)\tau(\gamma)\widetilde{\varphi}(y),\, \tau^{-1}(\gamma)\psi(x)\Big\rangle_{\mathcal{H}} \\
&= \int_M \mathrm{d}x \sum_{\gamma\in\Gamma} \Big\langle \int_M \mathrm{d}y\, K^*_A(x,y-\gamma)\varphi(y-\gamma),\, \psi(x)\Big\rangle_{\mathcal{H}} \\
&= \int_M \mathrm{d}x \Big\langle \int_{\mathbb{R}^d} \mathrm{d}y\, K^*_A(x,y)\varphi(y),\, \psi(x)\Big\rangle_{\mathcal{H}} \\
&= \int_M \mathrm{d}x\, \big\langle (\widehat{A^*}\varphi)(x),\, \psi(x)\big\rangle_{\mathcal{H}} = \big\langle \widehat{A^*}\varphi, \psi\big\rangle_{\mathcal{H}_\tau}
\end{aligned}$$

In particular, we used the τ-equivariance of the kernel (B.2) and of the functions in $\mathcal{H}_\tau$ and the unitarity of τ. By density we have $\widehat{A^*} = \widehat{A}^\dagger$. □

C Related approaches

This appendix collects some remarks to work which is closely related to space-adiabatic perturbation theory and which has partly been discussed already within the main body of this monograph.

C.1 Locally isospectral effective Hamiltonians

In adiabatic perturbation theory as described in this monograph the goal is to study the dynamics generated by the Hamiltonian

$$H^\varepsilon = H(x, -\mathrm{i}\varepsilon\nabla_x)$$

with operator valued symbol H by means of constructing effective Hamiltonians on certain approximately invariant subspaces.

However, the pioneering work of Born and Oppenheimer [BoOp] and most of the later work were dealing with the time-independent problem. Here the goal is the construction of an effective Hamiltonian which has the same spectrum as the full Hamiltonian H^ε, at least in some interval of the real line.

There are many rigorous results concluding this program for various physical systems. Most prominently time-independent Born-Oppenheimer approximation was rigorized in [CDS, KMSW] using the Grushin method for constructing locally isospectral effective Hamiltonians. The same idea was also applied to the Bloch electron in [GMS] and a considerably simplified presentation of the general method can be found in [Ma_2].

We will not enter in any technical details of this approach. But since it deals with essentially the same physical systems and since it appears to result in essentially the same effective Hamiltonians, it is important to clarify the differences.

To get a rough idea of the approach let us sketch the type of result one obtains in the following simple example. Let the spectrum of $H(q,p)$ consist of two eigenvalues $E_1(q,p)$ and $E_2(q,p)$ and continuous spectrum starting at $\Sigma(q,p)$, cf. Figure C.1. For energies λ in the interval $\Lambda_1 = (\inf E_1, \inf E_2)$ the construction yields an effective scalar Hamiltonian $H^\varepsilon_{\mathrm{eff}}(\lambda)$ with principal symbol $E_1(q,p)$. One has the following equivalence:

$$\lambda \in \sigma(H^\varepsilon) \quad \Leftrightarrow \quad \lambda \in \sigma(H^\varepsilon_{\mathrm{eff}}(\lambda))\,. \tag{C.1}$$

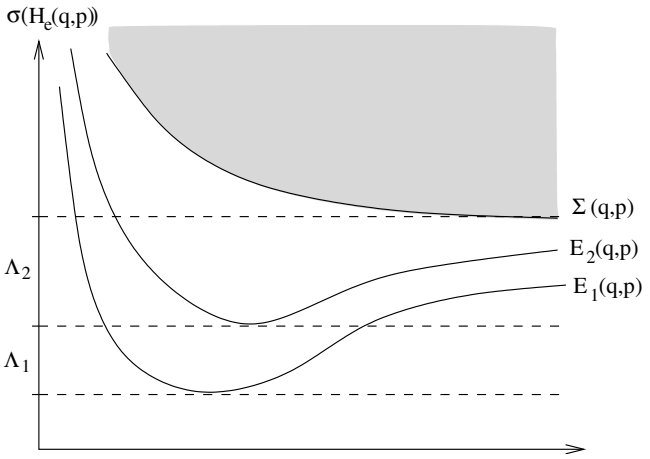

Fig. C.1. Schematic spectrum of a molecular Hamiltonian.

This means that a point $\lambda \in \Lambda_1$ is in the spectrum of the full Hamiltonian if and only if it is in the spectrum of the effective Hamiltonian. Furthermore, $H^{\varepsilon}_{\text{eff}}(\lambda)$ is a pseudodifferential operator and its principal symbol is just $E_1(q,p)$, i.e. it is given through Peierls' substitution. For values $\lambda \in (\inf E_2, \inf \Sigma)$ the same procedure works with the only difference that now $H^{\varepsilon}_{\text{eff}}(\lambda)$ is matrix-valued and contains E_1 and E_2 as well as their spectral projections. Once the continuous spectrum is reached the construction breaks down.

The isospectrality (C.1) is mathematically a very strong result. It is especially useful in the context of Born-Oppenheimer approximation as it allows for a perturbative study of the discrete spectrum of molecules. However, it gives almost no information about the dynamics.

We conclude that the two approaches, time-dependent and time-independent, give rather disjoint results. In the time-dependent setting we constructed subspaces of the full Hilbert space which are approximately invariant under time-evolution and on which the dynamics can be approximated by means of an effective Hamiltonian. In the time-independent setting to each energy one constructs an effective Hamiltonian which is isospectral to the original one.

Despite the differences, however, both approaches make use of the spectral structure of the symbol $H(q,p)$ and are, in particular, based on a gap condition. Both approaches yield an effective Hamiltonian starting with Peierl's substitution as the leading order term and agree, presumably, also at all higher orders.

C.2 Simultaneous adiabatic and semiclassical limit

As mentioned throughout the text, there are many other rigorous results available for time-dependent space-adiabatic problems.

The approach of Hagedorn [Ha$_1$, Ha$_3$, Ha$_4$, HaJo$_1$, HaJo$_2$] yields coherent state type solutions of the full Schrödinger equation (1.1), where the slow degrees of freedom are localized along some classical one-band trajectory and the fast degrees of freedom are approximately eigenstates of the corresponding eigenvalue band. The leading order results in the context of time-dependent Born-Oppenheimer approximation are sketched in Section 1.2.1. Recently Hagedorn and Joye [HaJo$_2$] succeeded in constructing exponentially accurate solutions of the full Schrödinger equation, which are still exponentially localized along the one-band classical trajectories. Moreover the approach of explicitly constructing solutions based on coherent states was extended to the case of eigenvalue crossings. In [Ha$_3$, Ha$_4$, HaJo$_1$] possible eigenvalue crossings in molecular dynamics are classified and solutions passing through the crossings are constructed. In particular the construction gives precise information on the transitions between otherwise isolated bands. This list of results shows that the approach based on coherent states is flexible and yields very precise results. The main drawback as compared to adiabatic perturbation theory—whenever the latter applies—is the restricted class of initial conditions and the fact that the adiabatic and the semiclassical limit are not separated. Hence in situations where quantum mechanical effects like tunnelling through small barriers or interference may still be observed, but adiabatic decoupling holds in good approximation, the coherent state approach is not applicable.

The time-dependent equation (1.1) with a Hamiltonian with a matrix-valued symbol was also discussed using matrix-valued Wigner measures. Under appropriate conditions the matrix valued Wigner transforms $W^\varepsilon(\psi^\varepsilon)$ of a sequence ψ^ε of initial wave functions converge weakly to some positive-matrix-valued measure on phase space. In [GMMP] it is shown that the diagonal elements of this measure (in an eigenbasis of the symbol of the Hamiltonian) satisfy classical transport equations, where the classical flow is generated by the eigenvalue bands of the symbol of the Hamiltonian. The advantage of this approach is that (presumably) less regularity of the symbols is needed. On the other hand only the leading order behavior is captured in the transport of the Wigner measures and the approach gives no control on the order of the errors. Again the adiabatic and the semiclassical limit are taken simultaneously. The Wigner function resp. Wigner measure approach was mostly used in the context of the Bloch electron [MMP, BFPR, BMP]. For a discussion how these results relate to resp. follow from the results of Chapter 5 we refer to [Te$_3$].

C.3 The work of Blount and of Littlejohn et al.

Within the physics literature effective Hamiltonians for certain space-adiabatic problems have been independently derived in a series of papers by Blount [Bl_1, Bl_2, Bl_3] in 1962 and later in a series of papers by Littlejohn, Flynn and Weigert [LiFl_1, LiFl_2, LiWe_1, LiWe_2] in the 90ties.

While Blount considers the problem of the Bloch electron [Bl_1, Bl_2] and the Dirac equation [Bl_3], Littlejohn et al. focus on Born-Oppenheimer type Hamiltonians [LiWe_1]. Whenever applicable, their techniques yield the same effective Hamiltonians as space-adiabatic perturbation theory. However, in the approach of Blount and of Littlejohn et. al. the full Hamiltonian is "diagonalized" at once. More precisely it is assumed that the spectrum of the symbol of the Hamiltonian consists only of globally isolated eigenvalue bands. Then a unitary operator is constructed such that the transformed Hamiltonian has a symbol which is a diagonal matrix at any order in ε. The clear advantage of space-adiabatic perturbation theory is that one can construct to any isolated band an effective Hamiltonian which approximates the full Hamiltonian on a certain almost invariant subspace. It is not required that all the spectrum consists of isolated bands, a condition which is not satisfied in most applications.

List of Symbols

General notation

$\mathcal{E}$	a Banach space
$\| \cdot \|_{\mathcal{E}}$	norm of the Banach space $\mathcal{E}$
$\mathcal{H}$	a separable Hilbert space
$\langle \cdot , \cdot \rangle_{\mathcal{H}}$	inner product of the Hilbert space $\mathcal{H}$
$\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$	Banach space of bounded linear operators $A : \mathcal{H}_1 \to \mathcal{H}_2$
A^*	adjoint operator in $\mathcal{L}(\mathcal{H}_2, \mathcal{H}_1)$ for $A \in \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$
$D(A)$	domain of an densely defined linear operator A on $\mathcal{H}$
$\sigma(A)$	spectrum of an operator A
$\mathrm{Tr} A$	trace of a trace-class operator A
$[A, B]$	commutator $[A, B] = AB - BA$ of two operators
$\mathbf{1}_{\mathcal{E}}$	identity operator on $\mathcal{E}$
$\mathbf{1}_{\Lambda}$	characteristic function of the set Λ
$\langle \cdot \rangle$	the function $\mathbb{R}^d \to [0, \infty)$, $x \mapsto \langle x \rangle = (1 + x^2)^{1/2}$
$\mathcal{O}(\varepsilon^n)$	a function $f : (0, \varepsilon_0] \to \mathcal{E}$ satisfies $f(\varepsilon) = \mathcal{O}(\varepsilon^n)$ iff there is a constant $C < \infty$ such that $\| f(\varepsilon) \| \leq C\varepsilon^n$.
$\mathcal{O}(\varepsilon^\infty)$	$f(\varepsilon) = \mathcal{O}(\varepsilon^\infty) \Leftrightarrow f(\varepsilon) = \mathcal{O}(\varepsilon^n)$ for all $n \in \mathbb{N}$.
$\asymp$	$f(\varepsilon) \asymp \sum_{n=0}^{\infty} \varepsilon^n a_n \Leftrightarrow \| f(\varepsilon) - \sum_{n=0}^{N} \varepsilon^n a_n \| = \mathcal{O}(\varepsilon^{N+1})$ $\forall N \in \mathbb{N}$
$\times$	Cartesian product of sets or vector product in $\mathbb{R}^3$

Function spaces

$C(\Omega, \mathcal{E})$	space of continuous functions on some domain $\Omega \subset \mathbb{R}^d$ with values in $\mathcal{E}$
$C^k_{\mathrm{b}}(\Omega, \mathcal{E})$	space of k-times continuously differentiable functions which are uniformly bounded together with all their derivatives
$C_0(\Omega, \mathcal{E})$	continuous functions with compact support
$\mathcal{S}(\mathbb{R}^d, \mathcal{H})$	Schwartz functions with values in $\mathcal{H}$
$\mathcal{S}'(\mathbb{R}^d, \mathcal{H})$	the dual space of $\mathcal{S}(\mathbb{R}^d, \mathcal{H})$
$L^p(\mathbb{R}^d, \mathcal{E})$	Lebesgue-Bochner spaces
H^k	Sobolev space of order k ($H^k = W^{k,2}$)

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Pseudodifferential calculus

$\widehat{A}$ or $\mathcal{W}^{\varepsilon}(A)$	Weyl quantization of the symbol A
$S^m_\rho(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$	space of symbols of order $m \in \mathbb{R}$ and weight $\rho \in [0,1]$ with values in $\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)$
$S^w(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$	space of symbols with order function w with values in $\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)$
$S^m_\rho(\varepsilon)$, $S^w(\varepsilon)$	spaces of semiclassical symbols
$M^m_\rho(\varepsilon)$, $M^w(\varepsilon)$	spaces of formal symbols (= formal power series)
K_A	integral kernel of the operator $\widehat{A}$
$(A_\varepsilon)_n$	n^{th} term in the asymptotic expansion of a semiclassical symbol A_ε
$\widetilde{\#}$	Weyl product $\widetilde{\#} : S^{m_1}_\rho(\varepsilon) \times S^{m_2}_\rho(\varepsilon) \to S^{m_1+m_2}_\rho(\varepsilon)$ respectively $\widetilde{\#} : S^{w_1}(\varepsilon) \times S^{w_2}(\varepsilon) \to S^{w_1 w_2}(\varepsilon)$
$\#$	Moyal product $\# : M^{m_1}_\rho(\varepsilon) \times M^{m_2}_\rho(\varepsilon) \to M^{m_1+m_2}_\rho(\varepsilon)$ respectively $\widetilde{\#} : M^{w_1}(\varepsilon) \times M^{w_2}(\varepsilon) \to M^{w_1 w_2}(\varepsilon)$
$\{\cdot,\cdot\}$	Poisson bracket
$\mathcal{O}_0(\varepsilon^\infty)$	see Definition A.17
$\mathcal{O}_{-\infty}(\varepsilon^\infty)$	see Definition A.16

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