Space-Adiabatic Perturbation Theory

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Abstract

We study approximate solutions to the Schrödinger equation $i\varepsilon\partial\psi_t(x)/\partial t = H(x, -i\varepsilon\nabla_x)\,\psi_t(x)$ with the Hamiltonian H the Weyl quantization of the symbol $H(q,p)$ taking values in the space of bounded operators on the Hilbert space $\mathcal{H}_{\mathrm{f}}$ of fast "internal" degrees of freedom. By assumption $H(q,p)$ has an isolated energy band. We prove that interband transitions are suppressed to any order in ε. As a consequence, associated to that energy band there exists a subspace of $L^2(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}})$ almost invariant under the unitary time evolution. We develop a systematic perturbation scheme for the computation of effective Hamiltonians which govern approximately the intraband time evolution. As examples for the general perturbation scheme we discuss the Dirac and Born-Oppenheimer type Hamiltonians and we reconsider also the time-adiabatic theory.

Contents

1 Introduction

Quantum theory has the remarkable feature that certain dynamical degrees of freedom may become “slaved” and thus lose their autonomous status. The origin of this phenomenon is a separation, both in space and time, into slow and fast degrees of freedom. The fast modes quickly adapt to the slow modes which in turn are governed by a suitable effective Hamiltonian. This mechanism is called adiabatic decoupling.

As paradigm we mention the motion of nuclei. The electronic degrees of freedom rapidly adjust to the state of lowest energy at given positions of the nuclei and the electronic energy band serves as effective potential in the Hamiltonian for the nuclei. This Born-Oppenheimer approximation is the basis for the dynamics of molecules and, as a consequence, also for the theory of classical fluids. There are many other examples of a similar structure. A very widely studied case are electrons moving in the periodic crystal potential, which defines the short scale. The envelope of the electronic wave function is governed by an effective Hamiltonian obtained from the Peierls substitution, in which the band energy is taken as effective kinetic energy. For an electron coupled to the quantized radiation field the photons are the fast degrees of freedom and the dynamics of the electron is governed by an effective Hamiltonian accounting for spin precession. These and other systems have been studied extensively by model specific approximate methods without realizing that they share a common structure. It is one aim of our work to explore this common structure and to convince the reader that for the determination of adiabatically decoupled subspaces and for the derivation of effective Hamiltonians a model independent strategy is in fact vastly superior to a case by case investigation.

Our claim is that all examples can be moulded into the generic form

$$i\varepsilon \frac{\partial}{\partial t}\psi_t(x) = H(x, -i\varepsilon\nabla_x)\psi_t(x)\,. \tag{1}$$

Here $H(q,p)$ is an operator-valued function on the classical phase space $\Gamma = \mathbb{R}^{2d}$ of the slow degrees of freedom with q a position like and p a momentum like variable. $H(q,p)$ is self-adjoint and acts on the Hilbert space $\mathcal{H}_\mathrm{f}$ of "internal" degrees of freedom. After quantization $H(x, -i\varepsilon\nabla_x)$ becomes the Hamiltonian of our system. To properly define it one has to specify an ordering of the operators $x, -i\varepsilon\nabla_x$, for which we will adopt the Weyl quantization rule as to be explained in full detail in Section 2. ψ_t is a wave function on $\mathbb{R}^d$ with values in $\mathcal{H}_\mathrm{f}$. Thus the quantum mechanical Hilbert space of states is $\mathcal{H} = L^2(\mathbb{R}^d, \mathcal{H}_\mathrm{f}) = L^2(\mathbb{R}^d) \otimes \mathcal{H}_\mathrm{f}$. Finally ε is a dimensionless parameter which controls the scale separation, $\varepsilon \ll 1$. Examples will be given in due course and we only remark that, in general, (1) is already the result of a proper identification of the slow degrees of freedom. For example, in nonrelativistic QED q stands for the position of the electron, whereas p is the total momentum of the electron and photons. For an electron in a periodic potential (1) is the Hamiltonian in the crystal momentum basis with x standing for the Bloch momentum k in the first Brillouin zone.

The origin of decoupling can be traced to a spectral property of $H(q,p)$. It is assumed, and it can be proved in many particular cases, that for each q, p the spectrum, $\sigma(q,p)$, of $H(q,p)$ can be decomposed into a "relevant" part $\sigma_\mathrm{r}(q,p)$ and a remainder in such a way that the relevant energy band $\{(q,p,\lambda) \in \mathbb{R}^{2d+1} : \lambda \in \sigma_\mathrm{r}(q,p)\}$ is separated from the remainder $\{(q,p,\lambda) \in \mathbb{R}^{2d+1} : \lambda \in \sigma_\mathrm{r}(q,p)^\mathrm{c}\}$ by a gap, i.e. by a corridor of finite width. Often the relevant part of the spectrum consists of a single, possibly degenerate eigenvalue. Then the relevant energy band would be the graph of a smooth function. Of course, a given $H(q,p)$ could have several such relevant energy bands and we suppose one of them to be singled out, e.g., through the initial condition. We will prove that the relevant energy band can be associated with an almost invariant subspace of $\mathcal{H}$ in such a way that if the initial wave function ψ_0 lies in that subspace then the solution ψ_t to (1) remains in that subspace up to errors which are small to any order of ε. The almost invariant subspace no longer communicates with the other parts of the system. Interband transitions are very much suppressed for small ε. In addition the intraband evolution can be approximated through some effective Hamiltonian at any desired precision in ε. In physical applications it is not uncommon to have the energy band, or a group of energy bands, separated by a gap only locally in q, p, which would then require a local version of the results discussed here. While this can be done, the rigorous realization of such a program would seriously cloud the simple ideas behind our constructions.

A Schrödinger equation in structure very similar to (1) appears in the time-adiabatic theorem of quantum mechanics. $H(q,p)$ is replaced by the time-dependent Hamiltonian $H(t)$ acting on $\mathcal{H}_\mathrm{f}$ and (1) becomes

$$i\varepsilon \frac{\partial}{\partial t}\psi(t) = H(t)\psi(t)\,. \tag{2}$$

The relevant energy band is now a function of t. If it is separated by a gap, the decoupling to all orders and effective Hamiltonians are well understood [Ka_1, ASY, JoPf, Ne_1]. Thus (1) may be regarded as the spatial version of the adiabatic theorem and one of our goals is to establish the general *space*-adiabatic theorem of quantum mechanics. In fact (2) results by inserting in (1) a prescribed classical trajectory q_t, p_t. While the internal degrees of freedom are treated quantum mechanically the orbital motion is regarded as classical. Physically it seems more natural to us to treat all degrees of freedom on the same footing. Hence (2) must be derived as a valid approximation.

The adiabatic decoupling is mostly taken for granted and the real task is considered to be the determination of effective Hamiltonians, for which model dependent techniques are employed. Thereby it is ignored that merely on the basis of (1) a computational scheme should be available. We like to compare this situation with standard perturbation theory for isolated eigenvalues. There is a general scheme available which is valid for any operator. Of course, the rich physics can be explored only in working out the answers in concrete cases. In this sense our second goal is to develop such a scheme for (1), which we call *space-adiabatic perturbation theory*. In principle this will be achieved to any order, but in practice the complexity very rapidly increases and it is hardly feasible to go beyond second order, except for rather special cases.

Our paper has become somewhat bulky for reasons which should be explained next. For the decoupling and the general construction of the effective Hamiltonians we need tools from the theory of pseudodifferential operators, which has a long tradition and which is extensively covered in the literature [Hö, Fo, DiSj, Ma]. Also certain less standard aspects of our work, like operator-valued symbols, have been well investigated. Still we found it difficult to give precise references on what is needed in our context. Therefore we decided, also for the convenience of the reader, to give a concise self-contained summary, quoting only readily available results. In this connection we stress that our ultimate goal are approximate solutions to the Schrödinger equation (1). Indeed our strongest results are approximations of the unitary propagator $\exp[-iH(x, -i\varepsilon\nabla_x)t]$ in the norm of bounded operators. In Section 2 we recall the conventional definition of symbol classes, the Weyl quantization, and the Moyal product. The precise assumptions on the Hamiltonian $H(q,p)$ are stated in the opening of Section 3, under which we then construct the almost invariant subspace for an isolated energy band of (1). Such a construction gives precise meaning to the adiabatic decoupling of certain dynamical degrees of freedom, but by itself yields no immediate information on the intraband evolution. This issue is taken up in Section 4 and 5 where we develop a scheme for computing effective Hamiltonians as operating on a fixed reference Hilbert space. E.g., if the energy band is ℓ-fold degenerate, the reference space would be $L^2(\mathbb{R}^d) \otimes \mathbb{C}^\ell$. Thus there are two elements which are required to obtain an approximate solution to (1): (i) the unitary evolution in the reference Hilbert space as generated by a suitable effective Hamiltonian, (ii) a unitary operator which maps the reference Hilbert space to the almost invariant subspace. The advantage of our construction is to have a clear separation between kinematics, as specified by the adiabatically decoupled subspace, and dynamics, defined through the effective Hamiltonian on the reference Hilbert space. The net result will be that for a given level of precision, $\varepsilon^n, n \geq 1$, there is a constructed approximate solution to (1) valid over a time scale $\varepsilon^{-k}t$, $k \geq 0$.

In the second half of our paper we work out more concretely the space-adiabatic perturbation theory. A reader less interested in the general constructions might in fact jump ahead directly to Section 5 after familiarizing himself with the few basic notions from Section 2. In Section 5 we provide the general formulae for the effective Hamiltonian and the unitary map up to order ε^2. To illustrate our scheme we determine the Born-Oppenheimer approximation including terms of order ε^2. The Born-Oppenheimer approximation is in some respects a rather simple example. Another easily accessible case is the time adiabatic theorem which by the Howland trick can be formulated also in the form (1) through a particular choice of H. Again all objects are given including order ε^2. The only physical example which is worked out in detail is the Dirac equation with slowly varying external potentials. In this case $\mathcal{H}_\mathrm{f} = \mathbb{C}^4$ and there are two two-fold degenerate energy bands, one for the electron and one for the positron. Thus the reference Hilbert space is $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$. The effective Hamiltonian is determined including order ε. It describes the translational motion through the Peierls substitution and the spin precession as governed by the BMT equation. Since the external vector potential enters through minimal coupling, the projection $P(q,p)$ on the electron subspace depends, in contrast to Born-Oppenheimer and time-dependent Hamiltonians, nontrivially on both coordinates. Thus the Dirac equation is one example where the full generality of our scheme is required.

The effective Hamiltonian still contains ε as a small parameter and is thus most conveniently analyzed through semiclassical methods. Typically their domain of validity is more restricted. In some earlier work the adiabatic and the semiclassical limit are lumped together, which has the disadvantage that the two sources of error are not clearly separated. For example for a relevant energy band with internal eigenvalue crossings, the adiabatic limit is still valid at any order, whereas the semiclassical analysis has to carefully treat the internal crossing. Such items are discussed in Section 6 including evolution equations for semiclassical observables. We also explain that beyond leading order the approximate semiclassical observable has to be determined from the context and is not given a priori. A summary of our results is listed in the final section.

We are not the first one to consider approximate solutions to (1) and special cases have been studied already in fair detail. To give an exhaustive discussion of the relevant literature is hardly feasible at this point and will be supplied later on. We only mention the remarkable work by E. I. Blount [Bl$_1$, Bl$_2$]. He remains on a purely formal level but, to our knowledge, for the first time understands the adiabatic problem (1) in the context of matrix-valued functions. Independently, Littlejohn et al. [LiFl, LiWe] used the same approach for the special case of Born-Oppenheimer Hamiltonians, which have the structure $H(q,p) = \frac{1}{2}p^2\mathbf{1} + V(q)$ with $\mathbf{1}$ the unit operator and $V(q)$ a matrix-valued function, see Section 5.3. Our own thinking has been influenced by G. Nenciu [Ne$_2$, NeSo], who stressed the role of almost invariant subspaces, and by a work of A. Martinez and V. Sordoni [MaSo]. However, while in [NeSo] and [MaSo] the emphasis lies on exponential error estimates, in our work we focus on *explicit* expansions to some finite order.

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2 Operator-valued Weyl calculus

Space-adiabatic perturbation theory deals with quantum systems in which it is possible to distinguish between fast and slow degrees of freedom. In particular we assume that the Hilbert space $\mathcal{H}$ admits a natural decomposition as $\mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathcal{H}_{\mathrm{f}}$, 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.

As the second structural ingredient we require that the Hamiltonian is given as the quantization of a $\mathcal{B}(\mathcal{H}_{\mathrm{f}})$-valued function on the classical phase space $\mathbb{R}^{2d}$ of the slow degrees of freedom. Hence we need to consider the generalization of the usual quantization rules to the case of $\mathcal{B}(\mathcal{H}_{\mathrm{f}})$-valued functions on $\mathbb{R}^{2d}$. This theory is well covered in the literature, see for example [Hö, Fo, Iv, GMS]. Still, for the convenience of the reader and to settle the notation, we prefer to provide a self-contained review of the basic results.

Notation. Let $\mathcal{E}$ be a Banach space. We will denote as $\mathcal{C}(\mathbb{R}^d, \mathcal{E})$ the space of $\mathcal{E}$-valued continuous functions on $\mathbb{R}^d$. In the same spirit we will employ the notation $\mathcal{S}(\mathbb{R}^d, \mathcal{E})$, $L^p(\mathbb{R}^d, \mathcal{E})$, $\mathcal{S}'(\mathbb{R}^d, \mathcal{E})$, with the obvious meaning. Note that, in the special case where $\mathcal{E} = \mathcal{H}_{\mathrm{f}}$ is an Hilbert space, one has $L^2(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}}) \cong L^2(\mathbb{R}^d) \otimes \mathcal{H}_{\mathrm{f}}$. The space of the bounded operators on $\mathcal{E}$ will be denoted as $\mathcal{B}(\mathcal{E})$.

2.1 Weyl quantization

Let A be a $\mathcal{B}(\mathcal{H}_{\mathrm{f}})$-valued rapidly decreasing smooth function on $\mathbb{R}^{2d}$, i.e. $A \in \mathcal{S}(\mathbb{R}^{2d}, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$. If we denote by $\mathcal{F}A$ the Fourier transform of A then, by Fourier inversion formula,

$$A(q,p) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} (\mathcal{F}A)(\eta, \xi) \; e^{i(\eta \cdot q + \xi \cdot p)} \; d\eta d\xi \,,$$

where the integral is a Bochner integral for $\mathcal{B}(\mathcal{H}_{\mathrm{f}})$-valued functions. This suggest to define an operator $\widehat{A} \in \mathcal{B}(\mathcal{H})$, called the **Weyl quantization** of A, by substituting $e^{i(\eta \cdot q + \xi \cdot p)}$ with $e^{i(\eta \cdot \widehat{q} + \xi \cdot \widehat{p})} \otimes 1_{\mathcal{H}_{\mathrm{f}}}$ where $\widehat{q}$ is multiplication by x and $\widehat{p} = -i\varepsilon \nabla_x$ in $L^2(\mathbb{R}^d)$. The exponential is defined by using the spectral theorem and it is explicitly given by

$$\left(e^{i(\eta \cdot \widehat{q} + \xi \cdot \widehat{p})} \psi \right)(x) = e^{i\varepsilon(\eta \cdot \xi)/2} e^{i\eta \cdot x} \psi(x + \varepsilon \xi) \qquad \text{for } \psi \in L^2(\mathbb{R}^d). \tag{3}$$

Thus

$$\widehat{A} = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} (\mathcal{F}A)(\eta, \xi) \;\; \left(e^{i(\eta \cdot \widehat{q} + \xi \cdot \widehat{p})} \otimes 1_{\mathcal{H}_{\mathrm{f}}} \right) d\eta d\xi \,, \tag{4}$$

and, in particular,

$$\|\widehat{A}\|_{\mathcal{B}(\mathcal{H})} \leq \frac{1}{(2\pi)^d} \int_{\mathbb{R}^{2d}} \|(\mathcal{F}A)(\eta, \xi)\|_{\mathcal{B}(\mathcal{H}_{\mathrm{f}})} \; d\eta d\xi \,,$$

which implies that $\widehat{A}$ belongs to $\mathcal{B}(\mathcal{H})$ provided the Fourier transform of A belongs to $L^1(\mathbb{R}^{2d}, \, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$. We will also use the notation $\mathcal{W}_\varepsilon(A) \equiv \widehat{A}$ in order to emphasize the ε -dependence.

Substituting (3) in (4) one obtains that for every $\psi \in \mathcal{S}(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}})$

$$(\widehat{A}\psi)(x) = \frac{1}{(2\pi\varepsilon)^d} \int_{\mathbb{R}^{2d}} A(\tfrac{1}{2}(x+y), \xi) \, e^{i\xi \cdot (x-y)/\varepsilon} \, \psi(y) \; d\xi dy, \tag{5}$$

i.e. $\widehat{A}$ is an integral operator with kernel

$$K_A(x,y) = \frac{1}{(2\pi\varepsilon)^d} \int_{\mathbb{R}^d} A(\tfrac{1}{2}(x+y),\xi)\; e^{i\xi\cdot(x-y)/\varepsilon}\; d\xi\,.$$

The kernel K_A is obtained from A by partial Fourier transformation followed by an invertible and measure-preserving change of variables. Since these operations can be performed whenever A is a tempered distribution, we obtain (part of) the following result (see [Fo] Theorem 1.30)

Proposition 2.1 *The map $\mathcal{W}_\varepsilon : \mathcal{S}(\mathbb{R}^{2d}, \mathcal{B}(\mathcal{H}_\mathrm{f})) \to \mathcal{B}(\mathcal{H})$ defined by (4) extends uniquely to a bijection from $\mathcal{S}'(\mathbb{R}^{2d}, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ to the space of continuous linear maps from $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_\mathrm{f})$ to $\mathcal{S}'(\mathbb{R}^d, \mathcal{H}_\mathrm{f})$.*

Then for every continuous linear map $T : \mathcal{S}(\mathbb{R}^d, \mathcal{H}_\mathrm{f}) \to \mathcal{S}'(\mathbb{R}^d,\, \mathcal{H}_\mathrm{f})$ there exists a unique $\mathrm{Symb}(T) \in \mathcal{S}'(\mathbb{R}^{2d}, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ such that $T = \mathcal{W}_\varepsilon(\mathrm{Symb}(T))$. We stress that, in general, $\mathrm{Symb}(T)$ will be ε-dependent. In this situation one says that $\mathrm{Symb}(T)$ is the **(Weyl) symbol** of T. In the same spirit, the elements of $\mathcal{S}'(\mathbb{R}^{2d}, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ are called *classical symbols*. The term hermitian symbol (resp. anti-hermitian, normal) will denote an hermitian (resp. anti-hermitian, normal) element of $\mathcal{S}'(\mathbb{R}^{2d}, \mathcal{B}(\mathcal{H}_\mathrm{f}))$.

Another interesting property of the Weyl map, is the correspondence between the adjoint of the classical symbol and the adjoint of its quantization. In order to fix notation, if T is a continuous linear map from $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_\mathrm{f})$ to $\mathcal{S}'(\mathbb{R}^d,\, \mathcal{H}_\mathrm{f})$, its adjoint $T^\dagger$ is the map from $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_\mathrm{f})$ to $\mathcal{S}'(\mathbb{R}^d, \mathcal{H}_\mathrm{f})$ defined by

$$\left\langle T^\dagger\varphi, \psi\right\rangle = \left\langle T\psi, \varphi\right\rangle^* \qquad \text{for } \psi,\varphi \in \mathcal{S}(\mathbb{R}^d, \mathcal{H}_\mathrm{f})$$

where $\langle\cdot,\cdot\rangle$ denotes the *sesquilinear* pairing between $\mathcal{S}'(\mathbb{R}^d,\, \mathcal{H}_\mathrm{f})$ and $\mathcal{S}(\mathbb{R}^d,\, \mathcal{H}_\mathrm{f})$. The adjoint of a (continuous) classical symbol is defined by taking pointwise the adjoint in $\mathcal{B}(\mathcal{H}_\mathrm{f})$. By duality one obtains an involution on all $\mathcal{S}'(\mathbb{R}^{2d},\, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ which will be denoted by *. Then

$$\mathcal{W}_\varepsilon(A^*) = \mathcal{W}_\varepsilon(A)^\dagger \tag{6}$$

for every classical symbol A. With this result in mind we will denote both the sides of (6) as $\widehat{A}^*$.

Symbol classes. The Weyl correspondence $\mathcal{W}_\varepsilon$, in the form given in Proposition 2.1, is too general to be really manageable. One restricts attention to some special classes of symbols and operators, focusing in particular to classes of operators whose elements can be composed with one other.

Definition 2.2 *A function $A \in C^\infty(\mathbb{R}^{2d}, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ belongs to the symbol class $S^m_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ (with $m \in \mathbb{R}$ and $0 \le \rho \le 1$) if for every $\alpha,\beta \in \mathbb{N}^d$ there exists a positive constant $C_{\alpha,\beta}$ such that*

$$\sup_{q\in\mathbb{R}^d} \left\| (\partial^\alpha_q \partial^\beta_p A)(q,p) \right\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} \le C_{\alpha,\beta}\;\; \langle p\rangle^{m-\rho|\beta|}$$

for every $p \in \mathbb{R}^d$, where $\langle p\rangle = (1+|p|^2)^{1/2}$.

The space $S^m_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ is a Fréchet space, whose topology can be defined by the (directed) family of semi-norms

$$\|A\|_k^{(m)} = \sup_{|\alpha|+|\beta|\le k} \sup_{q,p\in\mathbb{R}^d} \langle p\rangle^{-m+\rho|\beta|} \left\|(\partial_q^\alpha \partial_p^\beta A)(q,p)\right\|_{\mathcal{B}(\mathcal{H}_{\mathrm{f}})}, \qquad k\in\mathbb{N}. \tag{7}$$

The behavior of the symbol classes with respect to the pointwise product is very simple, as can be proved by using the Leibniz rule.

Proposition 2.3 *If $A \in S^{m_1}_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ and $B \in S^{m_2}_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$, then AB belongs to $S^{m_1+m_2}_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ for every $m_1, m_2 \in \mathbb{R}$.*

The behavior under pointwise inversion is described in the following proposition. For every $T\in\mathcal{B}(\mathcal{H}_{\mathrm{f}})$ let the internal spectral radius be $\rho_{\mathrm{int}}(T) := \inf\{|\lambda| : \lambda\in\sigma(T)\}$.

Proposition 2.4 *Assume that $A \in S^m_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ is a normal symbol which is elliptic, in the sense that there exists a constant C_0 such that*

$$\rho_{\mathrm{int}}(A(q,p)) \ge C_0\,\langle p\rangle^m \qquad \textit{for any}\;\; p\in\mathbb{R}^d\,.$$

Then the pointwise inverse A^{-1} exists and belongs to $S^{-m}_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$.

Proof. As a consequence of the spectral theorem (for bounded normal operators) one has

$$\left\|A^{-1}(q,p)\right\|_{\mathcal{B}(\mathcal{H}_{\mathrm{f}})} = \rho_{\mathrm{int}}(A(q,p))^{-1} \le C\,\langle p\rangle^{-m}\,.$$

Similar bounds on derivatives can be obtained by noticing that

$$\left\|\nabla_p(A^{-1})\right\|_{\mathcal{B}(\mathcal{H}_{\mathrm{f}})} = \left\|-A^{-1}(\nabla_p A)\;A^{-1}\right\|_{\mathcal{B}(\mathcal{H}_{\mathrm{f}})} \le C'\,\langle p\rangle^{-m-\rho}$$

and applying the chain rule. □

Given a symbol A in $S^m_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ the corresponding Weyl quantization $\widehat{A}$ maps $\mathcal{S}(\mathbb{R}^d,\mathcal{H}_{\mathrm{f}})$ continuously into itself and then extends to a continuous operator on $\mathcal{S}'(\mathbb{R}^d,\mathcal{H}_{\mathrm{f}})$. It is convenient to introduce a special notation for such classes of operators on $\mathcal{S}(\mathbb{R}^d,\mathcal{H}_{\mathrm{f}})$, called pseudodifferential operators,

$$OPS^m_\rho := \left\{\mathcal{W}_\varepsilon(A) :\; A\in S^m_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))\right\}.$$

In the following we will sometimes denote $S^m_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ simply as S^m_ρ and we will use the shorthand $S^m := S^m_0$. Notice that $S^m_\rho \subseteq S^m_{\rho'}$ for any $\rho\ge\rho'$.

If A belongs to $S^0(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ then the corresponding Weyl quantization is a *bounded* operator on $\mathcal{H} = L^2(\mathbb{R}^d,\mathcal{H}_{\mathrm{f}})$. The following proposition sharpens this statement (see [Fo], Theorem 2.73).

Notation. 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

$$\|A\|_{C^k_{\mathrm{b}}} := \sup_{|\alpha|\le k}\sup_{x\in\mathbb{R}^d} \|(\partial_x^\alpha A)(x)\|_{\mathcal{B}(\mathcal{H}_{\mathrm{f}})}$$

it is a Banach space.

Proposition 2.5 (Calderon-Vaillancourt) *There exists a constant $C_d < \infty$ such that for every $A \in C_{\mathrm{b}}^{2d+1}(\mathbb{R}^{2d}, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ one has*

$$\|\widehat{A}\|_{\mathcal{B}(\mathcal{H})} \leq C_d \sup_{|\alpha|+|\beta|\leq 2d+1} \sup_{q,p\in\mathbb{R}^d} \left\|(\partial_q^\alpha \partial_p^\beta A)(q,p)\right\|_{\mathcal{B}(\mathcal{H}_{\mathrm{f}})} = C_d \, \|A\|_{C_{\mathrm{b}}^{2d+1}} .$$

This implies, in particular, that the Weyl quantization, regarded as a map $\mathcal{W}_\varepsilon : S^0(\mathcal{B}(\mathcal{H}_{\mathrm{f}})) \to \mathcal{B}(\mathcal{H})$, is *continuous* with respect to the Fréchet topology on $S^0(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$.

2.2 The Weyl-Moyal product

One can define an associative product in the space of classical symbols which corresponds to the composition of the operators. Given $A, B \in S^m_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ we know that $\widehat{A}, \widehat{B}$ map $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}})$ into itself. Then $\widehat{A}\widehat{B}$ is still an operator on $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}})$ and – by using Proposition 2.1 – one concludes that there exists a unique ε-dependent symbol $\mathrm{Symb}(\widehat{A}\widehat{B}) =: A \,\tilde{\#}\, B \in \mathcal{S}'(\mathbb{R}^{2d}, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ such that

$$\mathcal{W}_\varepsilon(A)\mathcal{W}_\varepsilon(B) = \mathcal{W}_\varepsilon(A \,\tilde{\#}\, B).$$

The symbol $A \,\tilde{\#}\, B$ is called the **Weyl product** (or the twisted product) of the symbols A and B. The symbol classes $S^m_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ have a nice behavior with respect to the Weyl product, as stated in the following proposition (see [Fo], Theorem 2.47).

Proposition 2.6 *The map $(A, B) \mapsto A \,\tilde{\#}\, B$ is continuous from $S^{m_1}_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}})) \times S^{m_2}_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ to $S^{m_1+m_2}_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ for every $m_1, m_2 \in \mathbb{R}$ and $0 \leq \rho \leq 1$.*

In particular, $S^0_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ and $S^\infty_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}})) := \bigcup_{m\in\mathbb{R}} S^m_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ are algebras with respect to the Weyl product $\tilde{\#}$.

Since the product $A \,\tilde{\#}\, B$ 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 [DiSj, Ma, Fo, Hö]).

Definition 2.7 *A map $A : [0, \varepsilon_0) \to S^m_\rho, \varepsilon \mapsto A_\varepsilon$ is called a semiclassical symbol of order m and weight ρ if there exists a sequence $\{A_j\}_{j\in\mathbb{N}}$ with $A_j \in S^{m-j\rho}_\rho$ such that for every $n \in \mathbb{N}$ one has that $\left(A_\varepsilon - \sum_{j=0}^{n-1} \varepsilon^j A_j\right)$ belongs to $S^{m-n\rho}_\rho$* 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*

$$\left\| A_\varepsilon - \sum_{j=0}^{n-1} \varepsilon^j A_j \right\|_k^{(m-n\rho)} \leq C_{n,k}\, \varepsilon^n \,, \tag{8}$$

where $\|\ldots\|_k^{(m)}$ is the k-th Fréchet semi-norm in S^m_ρ, introduced in (7).

In the following A_0 and A_1 will be called the **principal symbol** and the **subprincipal symbol** of A. The space of semiclassical symbols of order m and weight ρ will be denoted as $S^m_\rho(\varepsilon)$. If condition (8) is fulfilled, one writes

$$A \asymp \sum_{j\geq 0} \varepsilon^j A_j \qquad \text{in } S^m_\rho(\varepsilon)$$

and one says that A is asymptotically equivalent to the series $\sum_{j\geq 0}\varepsilon^j A_j$ in $S^m_\rho(\varepsilon)$. If A is asymptotically equivalent to the series in which $A_j = 0$ for every $j \in \mathbb{N}$, we write $A = \mathcal{O}(\varepsilon^\infty)$. To be precise, we should write $A = \mathcal{O}(\varepsilon^\infty)$ in $S^m_\rho(\varepsilon)$, but the latter specification is omitted whenever it is unambiguous from the context.

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 (e.g. [Ma]).

Proposition 2.8 *Let be $\{A_j\}_{j\in\mathbb{N}}$ an arbitrary sequence such that $A_j \in S^{m-j\rho}_\rho$. Then there exists $A \in S^m_\rho(\varepsilon)$ such that $A \asymp \sum_{j\geq 0}\varepsilon^j A_j$ in $S^m_\rho(\varepsilon)$ and A 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 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 (see [Fo], Theorem 2.49).

Proposition 2.9 *If $A \asymp \sum_{j\geq 0}\varepsilon^j A_j$ in $S^{m_1}_\rho(\varepsilon)$ and $B \asymp \sum_{j\geq 0}\varepsilon^j B_j$ in $S^{m_2}_\rho(\varepsilon)$, then $A \,\#\, B \in S^{m_1+m_2}_\rho(\varepsilon)$ has an asymptotic expansion given by*

$$\left(A \,\tilde{\#}\, B\right)_k (q,p) = (2i)^{-k} \sum_{|\alpha|+|\beta|+j+l=k} \frac{(-1)^{|\alpha|}}{|\alpha|!|\beta|!} \left((\partial^\alpha_q \partial^\beta_p A_j)(\partial^\alpha_p \partial^\beta_q B_l)\right)(q,p) \tag{9}$$

where it is understood that $k, j, l \in \mathbb{N}$ and $\alpha, \beta \in \mathbb{N}^d$.

For example $(A \,\tilde{\#}\, B)_0$ is simply given by the pointwise product $A_0 B_0$ and

$$(A \,\tilde{\#}\, B)_1 = A_0 B_1 + A_1 B_0 - \frac{i}{2}\{A_0, B_0\}$$

where $\{\cdot,\cdot\}$ denotes the Poisson bracket on $S^\infty_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$, defined through

$$\{A, B\} = \sum_{j=1}^d \frac{\partial A}{\partial p_j}\frac{\partial B}{\partial q_j} - \frac{\partial A}{\partial q_j}\frac{\partial B}{\partial p_j}. \tag{10}$$

Notice that, 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. $A(z) = a(z)\mathbf{1}_{\mathcal{H}_{\mathrm{f}}}$.

As a consequence of the previous result, it is convenient to introduce the space of the formal power series with coefficients in $S^\infty_\rho(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$. This space, equipped with the associative product given by (9) and with the involution defined by taking the adjoint of every coefficient, will be called the **algebra of formal symbols** over $\mathcal{B}(\mathcal{H}_{\mathrm{f}})$. In particular we will denote as $M^m_\rho(\varepsilon)$ the subspace of the formal power series with a resummation in $S^m_\rho(\varepsilon)$, i.e.

$$M^m_\rho(\varepsilon) := \left\{ \sum_{j\geq 0}\varepsilon^j A_j \, : \, A_j \in S^{m-j\rho}_\rho \right\}.$$

In the context of formal power series, the product defined by (9) will be called the **Moyal product** and denoted simply as $\#$. Notice that $\#$ defines a map from $M^{m_1}_\rho(\varepsilon) \times M^{m_2}_\rho(\varepsilon)$ to $M^{m_1+m_2}_\rho(\varepsilon)$. The Moyal product can also be regarded as a map from $M^{m_1}_\rho(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}})) \times$

$M^{m_2}_\rho(\varepsilon, \mathcal{H}_\mathrm{f})$ to $M^{m_1+m_2}_\rho(\mathcal{H}_\mathrm{f})$, where in (9) the operator A and its derivatives act on the vector B and its derivatives.

To sum up the previous discussion, we wish to point out that one can prove statements on three levels: formal symbols (i.e. formal power series), semiclassical symbols, and operators on $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_\mathrm{f}) \subseteq L^2(\mathbb{R}^d, \mathcal{H}_\mathrm{f})$. A simple example illustrates the interplay between these levels. Suppose that two formal symbols $A \in M^{m_1}_\rho(\varepsilon)$ and $B \in M^{m_2}_\rho(\varepsilon)$ Moyal commute, i.e. $[A, B]_\# = A\#B - B\#A = 0$. Let $A_\varepsilon \in S^{m_1}_\rho(\varepsilon)$ and $B_\varepsilon \in S^{m_2}_\rho(\varepsilon)$ be any two resummations of A and, respectively, B. Since we know *a priori* (by Prop. 2.9) that the Weyl product $A_\varepsilon \,\tilde{\#}\, B_\varepsilon$ belongs to $S^{m_1+m_2}_\rho(\varepsilon)$ it follows that the Weyl commutator $[A_\varepsilon, B_\varepsilon]_{\tilde{\#}}$ is asymptotically close to zero in $S^{m_1+m_2}_\rho(\varepsilon)$, 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

$$\big\| [A_\varepsilon, B_\varepsilon]_{\tilde{\#}} \big\|^{(m_1+m_2-n\rho)}_k \leq C_{n,k}\ \varepsilon^n .$$

If $\rho > 0$ we obtain that definitely $m_1 + m_2 - n\rho \leq 0$ for some $n \in \mathbb{N}$ and then Prop. 2.5 assures that the operator commutator $[\widehat{A}_\varepsilon, \widehat{B}_\varepsilon]$ can be bounded in the $\mathcal{B}(\mathcal{H})$-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 and H^{q+r} 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

$$\Big\| [\widehat{A}_\varepsilon, \widehat{B}_\varepsilon] \Big\|_{\mathcal{B}(H^q, H^{q+r})} \leq C_{n,q,r}\, \varepsilon^n$$

for any $\varepsilon \in [0, \varepsilon_0)$, where H^q stands for $H^q(\mathbb{R}^d, \mathcal{H}_\mathrm{f})$. Notice that for $\rho = 0$ and $m_1 + m_2 =: m > 0$ it is not possible to conclude from $[A, B]_\# = 0$ that $[\widehat{A}_\varepsilon, \widehat{B}_\varepsilon]$ is a bounded operator, since it could happen – for example – that $[A_\varepsilon, B_\varepsilon]_{\tilde{\#}} = e^{-\frac{1}{\varepsilon}} p^m$, which is asymptotically close to zero in $S^m_\rho(\varepsilon)$. In the following we will use the same symbol for an element in $S^m_\rho(\varepsilon)$ and its expansion in $M^m_\rho(\varepsilon)$. As suggested by the preceding discussion, we introduce the following synthetic notation.

Notation. Let be A and B semiclassical symbols in $S^m_\rho(\varepsilon)$. We will say that $B = A + \mathcal{O}_{-\infty}(\varepsilon^\infty)$ if $B - A$ is asymptotically close to zero in $S^m_\rho(\varepsilon)$ for $\rho > 0$.

With a little abuse, we will employ the same notation for pseudodifferential operators too, i.e. we write $\widehat{B} = \widehat{A} + \mathcal{O}_{-\infty}(\varepsilon^\infty)$ if $B = A + \mathcal{O}_{-\infty}(\varepsilon^\infty)$. As noticed above this is a strong concept of closeness, since it implies that $\widehat{B} - \widehat{A}$ is a smoothing operator. Compare with the following weaker concept.

Notation. Let be R and S two (ε-dependent) operators on $\mathcal{H}$. We will say that $R = S + \mathcal{O}_0(\varepsilon^\infty)$ if for every $n \in \mathbb{N}$ there exists a constant C_n such that

$$\|R - S\|_{\mathcal{B}(\mathcal{H})} \leq C_n \varepsilon^n$$

for every $\varepsilon \in [0, \varepsilon_0)$. In such a case we will say that R is $\mathcal{O}_0(\varepsilon^\infty)$-close to S.

3 General setting and construction of the almost-invariant subspace

We are now in a position to state the general assumptions on which the adiabatic perturbation theory will be based in the following. Let $\mathcal{H}_{\mathrm{f}}$ be a separable Hilbert space, the state space for the fast degrees of freedom, and $\mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathcal{H}_{\mathrm{f}}$. The Hamiltonian $\widehat{H}$ of the full system is given as the Weyl quantization of a semiclassical symbol $H \in S^m_\rho(\varepsilon)$ and we assume that $\widehat{H}$ is essentially self-adjoint on $\mathcal{S}$. A point in the classical phase space $\mathbb{R}^{2d}$ is denoted by $z = (q,p) \in \mathbb{R}^{2d}$.

The adiabatic decoupling relies on a gap condition for the principal symbol H_0 of H.

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

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

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

$$\mathrm{dist}(\sigma(z) \setminus \sigma_{\mathrm{r}}(z), \mathrm{I}(z)) \geq C_g \langle p \rangle^\sigma ; \tag{11}$$

(G3) the width of the interval $\mathrm{I}(z)$ is uniformly bounded, i.e. $\sup_{z \in \mathbb{R}^{2d}} |\gamma_+(z) - \gamma_-(z)| \leq C < \infty$.

We denote the spectral projector corresponding to $\sigma_{\mathrm{r}}(z)$ by $\pi_0(z)$. As explained in the Introduction, one expects interband transitions to be suppressed for small ε. To prove such a property we need either one of the following assumptions to be satisfied.

Condition of increasing gap $(\mathbf{IG})_m$. Let H be an *hermitian* symbol in $S^m_\rho(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ (with $\rho > 0$ and $m \geq 0$) such that the principal symbol H_0 satisfies condition $(\mathrm{Gap})_\sigma$ with $\sigma = m$.

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

Note that for the case $H \in S^1_1(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ one can show that $\widehat{H}$ – the Weyl quantization of H – is essentially self-adjoint on the domain $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}}) \subseteq \mathcal{H}$. The proof is postponed to an appendix to the space-adiabatic theorem.

In analogy with the usual time-adiabatic theorem of quantum mechanics, see Section 5.4, we baptize the following result as *space-adiabatic theorem.* It establishes that there are almost invariant subspaces associated with isolated energy bands. In spirit the result is not new. However, to our knowledge it appears in this explicit form only recently 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 5.3) 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.

Theorem 3.1 (Space-adiabatic theorem) *Assume either (IG)$_m$ or (CG). Let $\widehat{H}$ be the Weyl quantization of H. Then there exists an orthogonal projector $\Pi \in \mathcal{B}(\mathcal{H})$ such that*

$$[\,\widehat{H},\,\Pi\,] = \mathcal{O}_0(\varepsilon^\infty) \tag{12}$$

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

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

whose principal part $\pi_0(z)$ is the spectral projector of $H_0(z)$ corresponding to $\sigma_{\mathrm{r}}(z)$.

The subspace $\mathrm{Ran}\Pi \subseteq \mathcal{H}$ is an almost invariant subspace for the dynamics generated by the Hamiltonian $\widehat{H}$, i.e. $[e^{-i\widehat{H}t}, \Pi] = \mathcal{O}_0(\varepsilon^\infty |t|)$, and it is associated with the spectral band $\sigma_{\mathrm{r}}(z)$. The terminology was borrowed from [Ne$_2$] although $\mathrm{Ran}\Pi$ is, in general, *not* an almost invariant subspace in the sense of [Ne$_2$], since Π need not have a limit as $\varepsilon \to 0$.

Proof. To clarify the scheme of its construction, we decompose the proof into two steps.
Step I. Construction of the Moyal projector
In general π_0 is not a projector in the Moyal algebra, i.e. $\pi_0 \,\#\, \pi_0 \neq \pi_0$. 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 [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].

Lemma 3.2 *Assume either (IG)$_m$ or (CG). Then there exists a* unique *formal symbol*

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

such that $\pi_0(z)$ is the spectral projector of $H_0(z)$ corresponding to $\sigma_{\mathrm{r}}(z)$, with the following properties:

(i) $\pi \,\#\, \pi = \pi$,

(ii) $\pi^* = \pi$,

(iii) $[\,H,\,\pi\,]_\# := H \,\#\, \pi - \pi \,\#\, H = 0$.

Proof. We give the proof under the assumption (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 $\sigma_{\mathrm{r}}(z) = \{E_{\mathrm{r}}(z)\}$ is an eigenvalue, which, at the same time, proves uniqueness of π in the general case. It follows basically the construction as given in [EmWe]. 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 $\sigma_{\mathrm{r}}(z) = \{E_{\mathrm{r}}(z)\}$ is much better suited for explicit computations than the general construction which will follow later on.

Note that $\pi_0 \# \pi_0 - \pi_0 = \mathcal{O}(\varepsilon)$ and $[H_0, \pi_0]_\# = \mathcal{O}(\varepsilon)$ and proceed by induction. Assume that we found $\pi^{(n)} = \sum_{j=0}^{n} \pi_j$ such that

$$\pi^{(n)} \# \pi^{(n)} - \pi^{(n)} = \varepsilon^{n+1} G_{n+1} + \mathcal{O}(\varepsilon^{n+2}) , \tag{13}$$

where, in particular, (13) defines G_{n+1}. Thus the next order term in the expansion π_{n+1} must satisfy

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

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

$$\pi_{n+1}^{\mathrm{D}} = -\pi_0\, G_{n+1}\, \pi_0 + (1-\pi_0)\, G_{n+1}\, (1-\pi_0) . \tag{14}$$

Since $G_{n+1} = \pi_0\, G_{n+1}\, \pi_0 + (1-\pi_0)\, G_{n+1}\, (1-\pi_0)$ follows from the fact that G_{n+1} is the principal symbol of $\varepsilon^{-n-1}(\pi^{(n)} \# \pi^{(n)} - \pi^{(n)})$, $\omega^{(n)} := \pi^{(n)} + \varepsilon^{n+1}\pi^{\mathrm{D}}_{n+1}$ indeed satisfies (i) up to an error of order $\mathcal{O}(\varepsilon^{n+2})$.

By induction assumption we also have that $[H, \pi^{(n)}]_\# = \mathcal{O}(\varepsilon^{n+1})$ and thus

$$[H, \omega^{(n)}]_\# = \varepsilon^{n+1} F_{n+1} + \mathcal{O}(\varepsilon^{n+2}) . \tag{15}$$

Hence, the diagonal part of π_{n+1} being fixed already, the off-diagonal part of π_{n+1} must satisfy $[H_0, \pi^{\mathrm{OD}}_{n+1}] = -F_{n+1}$. In particular,

$$\begin{aligned} H_0(z)\ (\pi_0(z)\pi_{n+1}(z)(1-\pi_0(z))) - (\pi_0(z)\pi_{n+1}(z)(1-\pi_0(z)))\ H_0(z) & \\ = -\,\pi_0(z)\, F_{n+1}(z)\, (1-\pi_0(z)) & \end{aligned} \tag{16}$$

for all $z \in \mathbb{R}^{2d}$. We first show that if (16) has a solution $\pi_0(z)\pi_{n+1}(z)(1-\pi_0(z)) =: \pi^{OD1}_{n+1}(z)$, it is unique, i.e. that the kernel of the map $\pi^{OD1}_{n+1}(z) \mapsto [H_0(z), \pi^{OD1}_{n+1}(z)]$ restricted to $\mathrm{Ran}(1-\pi_0(z))$ contains only zero. To see this let $\overline{\sigma}_{\mathrm{r}}(z) := (\sup \sigma_{\mathrm{r}}(z) - \inf \sigma_{\mathrm{r}}(z))/2$ and note that, due to the gap condition, $H_0(z) - \overline{\sigma}_{\mathrm{r}}(z)$ is invertible on $\mathrm{Ran}(1-\pi_0(z))$ with $\|(H_0(z) - \overline{\sigma}_{\mathrm{r}}(z))^{-1}(1-\pi_0(z))\| < 2/\mathrm{diam}(\sigma_{\mathrm{r}}(z))$. Hence

$$\begin{aligned} [H_0(z), \pi^{OD1}_{n+1}(z)] = 0 &\Leftrightarrow [H_0(z) - \overline{\sigma}_{\mathrm{r}}(z), \pi^{OD1}_{n+1}(z)] = 0 \\ &\Leftrightarrow \ \pi^{OD1}_{n+1}(z) = (H_0(z) - \overline{\sigma}_{\mathrm{r}}(z))\pi^{OD1}_{n+1}(z)(H_0(z) - \overline{\sigma}_{\mathrm{r}}(z))^{-1} \end{aligned}$$

and therefore

$$\begin{aligned} \|\pi^{OD1}_{n+1}(z)\| &\leq \|(H_0(z) - \overline{\sigma}_{\mathrm{r}}(z))\pi_0(z)\|\, \|\pi^{OD1}_{n+1}(z)\|\, \|(H_0(z) - \overline{\sigma}_{\mathrm{r}}(z))^{-1}(1-\pi_0(z))\| \\ &= C\, \|\pi^{OD1}_{n+1}(z)\| \end{aligned}$$

with $C < 1$. Hence $\pi^{OD1}_{n+1}(z) = 0$ and we conclude that π_{n+1} is unique when it exists.

In the special case that $\sigma_{\mathrm{r}}(z) = \{E_{\mathrm{r}}(z)\}$, (16) can be solved, and one finds

$$\pi_0\pi_{n+1}(1-\pi_0) = \pi_0\, F_{n+1}\, (H_0 - E_{\mathrm{r}})^{-1}\, (1-\pi_0) . \tag{17}$$

Using that F_{n+1} is the principal symbol of $\varepsilon^{-n-1}[H, \omega^{(n)}]_\#$, 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 (14) and (17) satisfies (i) and (iii) up to $\mathcal{O}(\varepsilon^{n+2})$.

We conclude that by induction we have uniqueness of π in the general case, and an explicit construction for π when $\sigma_{\rm r}(z) = \{E_{\rm r}(z)\}$. The latter one involves four steps at each order: [a] Evaluation of G_{n+1} as in (13), [b] computation of $\pi^{\rm D}_{n+1}$ as in (14), [c] evaluation of F_{n+1} as in (15), [d] computation of $\pi^{\rm OD}_{n+1}$ as in (17).

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 $\sigma_{\rm r}(z)$ 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,

$$\mathrm{dist}(\Gamma(z_0), \sigma(z)) \geq \frac{1}{4} C_g \langle p \rangle^{\sigma} \qquad \text{for all } z \in \mathcal{U}_{z_0} \tag{18}$$

and

$$\mathrm{Radius}(\Gamma(z_0)) \leq C_{\rm r} \sup_{z \in \mathcal{U}_{z_0}} \langle p \rangle^{\sigma}, \tag{19}$$

where Radius$(\Gamma(z_0))$ is the radius of the complex circle $\Gamma = \Gamma(z_0)$. The constant C_g in (18) is the same as in (11) and the existence of a constant $C_{\rm r}$ *independent* of z_0 such that (19) is satisfied follows from assumption (G3). We keep σ in the notation as a bookkeeping device, in order to distinguish the contributions related to the gap, although $\sigma = m$.

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

$$R(\zeta) \# (H - \zeta 1) = 1 = (H - \zeta 1) \# R(\zeta) \qquad \text{on } \mathcal{U}_{z_0}. \tag{20}$$

The symbol $R(\zeta)$ can be explicitly constructed. We abbreviate

$$R_0(\zeta) \;=\; (H_0 - \zeta 1)^{-1}$$

where the inverse is understood in the $\mathcal{B}(\mathcal{H}_{\rm f})$-sense and exists according to (18). By induction, suppose that $R_{(n)}(\zeta) = \sum_{j=0}^{n} \varepsilon^j R_j(\zeta)$ satisfies the first equality in (20) up to $\mathcal{O}(\varepsilon^{n+1})$-terms, i.e.

$$R^{(n)}(\zeta) \# (H - \zeta 1) = 1 + \varepsilon^{n+1} E_{n+1}(\zeta) + \mathcal{O}(\varepsilon^{n+2}).$$

By choosing $R_{n+1} = -E_{n+1}\,(H_0 - \zeta 1)^{-1}$, we obtain that $R^{(n+1)} = R^{(n)} + \varepsilon^{n+1} R_{n+1}$ satisfies the same equality up to $\mathcal{O}(\varepsilon^{n+2})$-terms. Then the formal symbol $R(\zeta) = \sum_{j \geq 0} \varepsilon^j R_j(\zeta)$ satisfies the first equality in (20) which – by the associativity of the Moyal product – implies the second one.

Equation (20) implies that $R(\zeta)$ satisfies the *resolvent equation*

$$R(\zeta) - R(\zeta') = (\zeta - \zeta')\, R(\zeta) \# R(\zeta') \qquad \text{on } \mathcal{U}_{z_0}. \tag{21}$$

From the resolvent equation it follows – by using an argument similar to the standard one in operator theory [Ka] – that the symbol $\pi = \sum_{j \geq 0} \varepsilon^j \pi_j$ defined by

$$\pi_j(z) := \frac{i}{2\pi} \int_{\Gamma} R_j(\zeta, z)\, d\zeta, \qquad z \in \mathcal{U}_{z_0}, \tag{22}$$

is a Moyal projector such that $[H,\pi]_{\#}=0$ 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 (22) and we obtain

$$\begin{aligned}
(\pi\,\#\,\pi)_j &= \left(\frac{i}{2\pi}\right)^2\int_{\Gamma'}d\zeta'\int_{\Gamma}d\zeta\,\left(R(\zeta')\,\#\,R(\zeta)\right)_j \\
&= \left(\frac{i}{2\pi}\right)^2\int_{\Gamma'}d\zeta'\int_{\Gamma}d\zeta\,(\zeta'-\zeta)^{-1}\left[R(\zeta')-R(\zeta)\right]_j \\
&= \frac{i}{2\pi}\int_{\Gamma}R_j(\zeta)\;d\zeta=\pi_j
\end{aligned}\tag{23}$$

where (21) has been used. The first equality in (23) follows by noticing that for every $\gamma\in\mathbb{N}^{2d}$

$$\partial_z^\gamma\pi_j(z)=\frac{i}{2\pi}\int_\Gamma\partial_z^\gamma R_j(\zeta,z)\;d\zeta\qquad z\in\mathcal{U}_{z_0},$$

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 (20). From (22) it follows that π Moyal-commutes with $R(\lambda)$ for any $\lambda\in\Gamma$. Then, by multiplying $\pi\,\#\,R(\lambda)=R(\lambda)\,\#\,\pi$ by $(H-\lambda 1)$ on both sides, one obtains that $H\,\#\,\pi=\pi\,\#\,H$.

Finally we have to show that $\pi_j\in S_\rho^{-j\rho}$ for every $j\in\mathbb{N}$. From the Riesz formula (22) it follows that for every $\gamma\in\mathbb{N}^{2d}$ one has

$$\left\|(\partial_z^\gamma\pi_j)(z)\right\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})}\le 2\pi\ \mathrm{Radius}\left(\Gamma(z_0)\right)\sup_{\zeta\in\Gamma(z_0)}\left\|(\partial_z^\gamma R_j)(\zeta,z)\right\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})}.$$

According to (19) we are left to prove that

$$\sup_{\zeta\in\Gamma(z_0)}\left\|\left(\partial_q^\alpha\partial_p^\beta R_j\right)(\zeta,z)\right\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})}\le C_{\alpha\beta j}\,\langle p\rangle^{-\sigma-j\rho-|\beta|\rho},\qquad \alpha,\beta\,\in\mathbb{N}^d\,,\ j\in\mathbb{N},\tag{24}$$

where $C_{\alpha\beta j}$ must *not* depend on z_0. As for R_0, we notice that according to (18) one has

$$\left\|(H_0(z)-\zeta 1)^{-1}\right\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})}\le\frac{1}{\mathrm{dist}(\zeta,\sigma(H_0(z)))}\le\frac{4}{C_g}\,\langle p\rangle^{-\sigma},\tag{25}$$

and moreover,

$$\begin{aligned}
\left\|\nabla_p R_0(z)\right\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} &= \left\|-(R_0\nabla_pH_0R_0)(z)\right\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})}\le\left(\frac{4}{C_g}\right)^2\langle p\rangle^{-2\sigma}\left\|\nabla_pH_0(z)\right\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} \\
&\le C\,\langle p\rangle^{-2\sigma+m-\rho}=C\,\langle p\rangle^{-\sigma-\rho},
\end{aligned}$$

where the last bound follows from the fact that $H_0\in S_\rho^m$ (recall that $\sigma=m$). By induction one controls higher order derivatives and (24) follows for $j=0$.
Again by induction, assume that $R_0,\dots,R_n$ satisfy the bound (24). Then, by writing out

$$E_{n+1}=\left(R_{(n)}(\zeta)\,\#\,(H-\zeta 1)-1\right)_{n+1}$$

and using (9), one concludes that $R_{n+1} = -E_{n+1}R_0$ satisfies (24) with $\sigma = m$. □

Step II. Quantization
First of all, by resummation (Prop. 2.8) we obtain a semiclassical symbol $\pi : \mathbb{R}^{2d} \times [0, \varepsilon_0) \to \mathcal{B}(\mathcal{H}_\mathrm{f})$ whose asymptotic expansion is given by $\sum_{j\geq 0} \varepsilon^j \pi_j$. Then, by Weyl quantization, one gets a bounded operator $\widehat{\pi} \in \mathcal{B}(\mathcal{H})$ (see Prop. 2.5) 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) $[\widehat{H}, \widehat{\pi}] = \mathcal{O}_{-\infty}(\varepsilon^\infty)$

Notice that the assumption $\rho > 0$ is crucial in order to obtain (iii) for an unbounded $\widehat{H}$.

In order to get a true projector we follow the idea of [NeSo] and notice that $\|\widehat{\pi}^2 - \widehat{\pi}\| = \mathcal{O}(\varepsilon^\infty)$ and the spectral mapping theorem for self-adjoint operators imply that for each $n \in \mathbb{N}$ there is a $C_n < \infty$ such that

$$\sigma(\widehat{\pi}) \subset [-C_n\varepsilon^n, C_n\varepsilon^n] \cup [1 - C_n\varepsilon^n, 1 + C_n\varepsilon^n] =: \sigma_0^\varepsilon \cup \sigma_1^\varepsilon\,.$$

Hence one can define for $\varepsilon \leq 1/(4C_1)$

$$\Pi := \frac{i}{2\pi}\int_{|\zeta-1|=\frac{1}{2}} (\widehat{\pi} - \zeta)^{-1}\, d\zeta\,.$$

Then $\Pi^2 = \Pi$ follows and we claim that $\Pi = \widehat{\pi} + \mathcal{O}_0(\varepsilon^\infty)$. Indeed,

$$\widehat{\pi} = \int_{\sigma_0^\varepsilon \cup \sigma_1^\varepsilon} \lambda E(d\lambda) = \mathcal{O}_0(\varepsilon^n) + \int_{\sigma_1^\varepsilon} E(d\lambda) = \Pi + \mathcal{O}_0(\varepsilon^n) \qquad \text{for all } n \in \mathbb{N},$$

where $E(\cdot)$ is the projection valued measure of $\widehat{\pi}$. Finally notice that

$$\begin{aligned} [\widehat{H}, \Pi] &= \frac{i}{2\pi}\int_{|\zeta-1|=\frac{1}{2}} [\widehat{H}, (\widehat{\pi} - \zeta)^{-1}] d\zeta \\ &= -\frac{i}{2\pi}\int_{|\zeta-1|=\frac{1}{2}} (\widehat{\pi} - \zeta)^{-1} [\,\widehat{H}, \widehat{\pi}\,] (\widehat{\pi} - \zeta)^{-1} d\zeta\,, \end{aligned}$$

which implies that

$$\|[\widehat{H}, \Pi]\|_{\mathcal{B}(\mathcal{H})} \leq C\|[\widehat{H}, \widehat{\pi}]\|_{\mathcal{B}(\mathcal{H})} = \mathcal{O}_0(\varepsilon^\infty)\,.$$

This concludes the proof of the theorem. □

Essential self-adjointness of $\widehat{H}$.
Since H is an *hermitian* symbol its Weyl quantization $\widehat{H}$ is symmetric on the invariant domain $\mathcal{S}(\mathbb{R}^d, \mathcal{B}(\mathcal{H}_\mathrm{f})) \subseteq \mathcal{H}$. If H belongs to $S^0(\varepsilon)$ then $\widehat{H}$ is a bounded operator, and there is nothing to prove.

In order to prove essential self-adjointness in the case $H \in S^1_1(\varepsilon)$, we use an argument of [Ro]. The proof does not exploit the smallness of ε and we therefore consider any $\varepsilon > 0$. For $s > 0$ let

$$B_{\pm s}(q,p) = (H_0(q,p) \pm is1)^{-1}\,,$$

which, according to Proposition 2.4, belongs to $S^0_1(\mathcal{B}(\mathcal{H}_\mathrm{f}))$. Moreover

$$(H \pm is1) \,\tilde{\#}\, B_{\pm s} = \mathbf{1} + \varepsilon S_{\pm s}\,,$$

where $S_{\pm s} \in S^0_1(\varepsilon)$, since $H \in S^1_1(\varepsilon)$ and $B_{\pm s} \in S^0_1(\varepsilon)$. After Weyl quantization we obtain that

$$(\widehat{H} \pm is\mathbf{1})\; \widehat{B}_{\pm s} = \mathbf{1} + \varepsilon \widehat{S}_{\pm s} \qquad \text{with} \;\; \|\widehat{S}_{\pm s}\|_{\mathcal{B}(\mathcal{H})} < \frac{C}{|s|},$$

the latter bound following (for s large enough) from Proposition 2.5 and from estimating the Fréchet semi-norms of $S_{\pm s}$. Essential self-adjointness of $\widehat{H}$ on the domain $\mathcal{S}$ follows, if we can show that $\mathrm{Ker}(\widehat{H}^* \pm is) = \{0\}$ for some $s > 0$. For this let $\varphi \in \mathrm{Ker}(\widehat{H}^* \pm is)$ and $\psi \in \mathcal{S}$. Using $\widehat{B}_\pm \mathcal{S} \subset \mathcal{S}$, we obtain

$$0 = \langle (\widehat{H}^* \mp is)\varphi, \widehat{B}_\pm \psi\rangle = \langle \varphi, (\widehat{H} \pm is)\widehat{B}_\pm\psi\rangle = \langle \varphi, (\mathbf{1} + \varepsilon\widehat{S}_{\pm s})\psi\rangle\,.$$

Since $\|\varepsilon \widehat{S}_{\pm s}\| < 1$ for s large enough, $(\mathbf{1} + \varepsilon\widehat{S}_{\pm s})\mathcal{S}$ is dense in $\mathcal{H}$ and hence $\varphi = 0$ follows.

4 Reference subspace and intertwining unitaries

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 $\mathrm{Ran}\Pi$? The main obstruction for such a simple description is the fact that the subspace $\mathrm{Ran}\Pi$ depends on ε and is not easily accessible. Even worse, in general the limit $\lim_{\varepsilon\to 0}\Pi$ does not exist, meaning that $\mathrm{Ran}\Pi$ 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 $\mathrm{Ran}\Pi$ to an easily accessible and ε-independent *reference* subspace.

From the continuity of $z \mapsto H_0(z)$ and the gap condition it follows that there is a subspace $\mathcal{K}_\mathrm{f} \subset \mathcal{H}_\mathrm{f}$ independent of (q,p) such that the subspaces $\mathrm{Ran}\pi_0(q,p)$ are all isomorphic to $\mathcal{K}_\mathrm{f}$. Let π_r be the projection on $\mathcal{K}_\mathrm{f}$, then $\Pi_\mathrm{r} := \mathbf{1}\otimes\pi_\mathrm{r}$ $(= \widehat{\pi}_\mathrm{r})$ will serve as the projector on the *reference subspace* $\mathcal{K} := \mathrm{Ran}\Pi_\mathrm{r}$. Of course $\mathcal{K}_\mathrm{f}$ is *highly* non-unique and a convenient choice must be made in concrete applications.

Once the reference Hilbert space is fixed we next chose a unitary operator valued smooth function $u_0(z)$ which pointwise in phase space intertwines $\pi_0(z)$ and π_r, i.e.

$$u_0(z)^*\pi_0(z)\; u_0(z) = \pi_\mathrm{r}\,. \tag{26}$$

The existence of such a *smooth* map follows from a bundle-theoretic argument given at the end of this section. Again $u_0(z)$ is not unique and must be chosen conveniently. We will see in Section 7 that there is an optimal choice for $u_0(z)$, which reflects the physics of the problem.

Unfortunately we cannot prove that it is possible to choose u_0 in $S^0_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$. Indeed, relation (26) 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 u_0 is in $S^0_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$, as will be the case in the physical examples.

In the following $\mathcal{U}(\mathcal{H})$ will denote the group of unitary operators over $\mathcal{H}$.

Theorem 4.1 *Assume either (IG)$_m$ or (CG) and that there exists a $\mathcal{U}(\mathcal{H}_\mathrm{f})$-valued map $u_0 \in S^0_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ which satisfies (26). Then there exist a unitary operator $U \in \mathcal{B}(\mathcal{H})$ such that*

$$U^* \,\Pi\, U = \Pi_\mathrm{r} \tag{27}$$

and $U = \widehat{u} + \mathcal{O}_0(\varepsilon^\infty)$, where $u \asymp \sum_{j\geq 0} \varepsilon^j u_j$ in $S^0_\rho(\varepsilon)$ with principal symbol u_0.

Step I. Construction of the Moyal unitaries.
Again u_0 fails to be a Moyal unitary (i.e. $u_0^* \# u_0 \neq 1$) 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 pseudor has a long tradition, cf. [Ni] Section 7 and references therein, and was applied in different settings many times, e.g. [Ta, HeSj].

Lemma 4.2 *Assume either (IG)$_m$ or (CG) and that there exists a $\mathcal{U}(\mathcal{H}_\mathrm{f})$-valued map $u_0 \in S^0_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ which satisfies (26). Then there is a formal symbol $u = \sum_{j\geq 0} \varepsilon^j u_j$, with $u_j \in S^{-j\rho}_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$, such that*

(i) $u^* \# u = 1$ *and* $u \# u^* = 1\,,$

(ii) $u^* \# \pi \# u = \pi_\mathrm{r}\,,$

where π is the Moyal projector constructed in Lemma 3.2.

Remark 4.3 We emphasize that – as opposed to the Moyal projector π appearing in Lemma 3.2 – 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 parametrized by the antihermitian Moyal symbols which are diagonal in the π_r-splitting.

Proof of Lemma 4.2. 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

$$u_{n+1} =: u_0(a_{n+1} + b_{n+1})\,,$$

with a_{n+1} hermitian and b_{n+1} anti-hermitian. By induction assumption we have

$$\begin{aligned} u^{(n)*} \# u^{(n)} - 1 &= \varepsilon^{n+1} A_{n+1} + \mathcal{O}(\varepsilon^{n+2}) \\ u^{(n)} \# u^{(n)*} - 1 &= \varepsilon^{n+1} \tilde{A}_{n+1} + \mathcal{O}(\varepsilon^{n+2})\,. \end{aligned}$$

Thus u_{n+1} has to solve

$$\begin{aligned} u_0^*\, u_{n+1} + u_{n+1}^*\, u_0 &= -A_{n+1}, \\ u_{n+1}\, u_0^* + u_0\, u_{n+1}^* &= -\tilde{A}_{n+1}\,. \end{aligned} \tag{28}$$

The first equation in (28) fixes $a_{n+1} = -\frac{1}{2}A_{n+1}$, since A_{n+1} is hermitian as it is the principal symbol of $\varepsilon^{-n-1}(u^{(n)*} \# u^{(n)} - 1)$. The second equation in (28) is then also satisfied, since the compatibility equation $u_0\, A_{n+1} = \tilde{A}_{n+1}\, u_0$ follows from

$$\frac{1}{\varepsilon^{n+1}} u^{(n)} \# (u^{(n)*} \# u^{(n)} - 1) = \frac{1}{\varepsilon^{n+1}} (u^{(n)} \# u^{(n)*} - 1) \# u^{(n)}$$

by noticing that $u_0\, A_{n+1}$ (resp. $\tilde{A}_{n+1}\, u_0$) is the principal symbol of the l.h.s (resp. r.h.s).

Note that (28) puts no constraint on b_{n+1} and we are left to determine it using (ii). Let $w^{(n)} = u^{(n)} + \varepsilon^{n+1} u_0 a_{n+1}$, then by induction assumption

$$w^{(n)*} \# \pi \# w^{(n)} - \pi_{\mathrm{r}} = \varepsilon^{n+1} B_{n+1} + \mathcal{O}(\varepsilon^{n+2})$$

and thus

$$u^{(n+1)*} \# \pi \# u^{(n+1)} - \pi_{\mathrm{r}} = \varepsilon^{n+1} \left(B_{n+1} - [b_{n+1}, \pi_{\mathrm{r}}]\right) + \mathcal{O}(\varepsilon^{n+2})\,.$$

Hence we need to find an anti-hermitian b_{n+1} satisfying

$$B_{n+1} - [b_{n+1}, \pi_{\mathrm{r}}] = 0\,,$$

which is given by

$$b_{n+1} = [B_{n+1}, \pi_{\mathrm{r}}], \tag{29}$$

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 $\varepsilon^{-(n+1)}\left(w^{(n)*} \;\#\; \pi \;\#\; w^{(n)} - \pi_{\mathrm{r}}\right)$ and then

$$\begin{aligned}
&(1-\pi_{\mathrm{r}})\; B_{n+1}\; (1-\pi_{\mathrm{r}}) \overset{\varepsilon\to 0}{\sim} \frac{1}{\varepsilon^{n+1}}(1-\pi_{\mathrm{r}})\left(w^{(n)*} \;\#\; \pi \,\#\; w^{(n)} - \pi_{\mathrm{r}}\right)\; (1-\pi_{\mathrm{r}}) \\
= \;& \frac{1}{\varepsilon^{n+1}}(1-\pi_{\mathrm{r}})\left(w^{(n)*} \;\#\; \pi \;\#\; w^{(n)}\right)(1-\pi_{\mathrm{r}}) \\
= \;& \frac{1}{\varepsilon^{n+1}}\left(\varepsilon^{2(n+1)} B_{n+1} \left(w^{(n)*} \;\#\; \pi \,\#\; w^{(n)}\right) B_{n+1} + \mathcal{O}(\varepsilon^{n+2})\right) \overset{\varepsilon\to 0}{\sim} 0,
\end{aligned}$$

where for the last equality we inserted $1-\pi_{\mathrm{r}} = w^{(n)*} \# (1-\pi) \# w^{(n)} + \varepsilon^{n+1} B_{n+1} + \mathcal{O}(\varepsilon^{n+2})$ 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 (29) 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 4.3.

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

$$a_{n+1} = -\frac{1}{2}A_{n+1} = -\frac{1}{2}\left(u^{(n)*} \# u^{(n)} - 1\right)_{n+1}$$

shows that a_{n+1} belongs to $S^{-(n+1)\rho}_\rho$ as it is the $(n+1)$-th term of an element of $M^0_\rho(\varepsilon)$. By Proposition 2.3, $u_0 a_{n+1} \in S^{-(n+1)\rho}_\rho$ 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 $u_0 b_{n+1} \in S^{-(n+1)\rho}_\rho$, 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 $S^0_\rho(\varepsilon)$ (see Prop. 2.8). Then, by Weyl quantization, one gets a bounded operator $\widehat{u} \in \mathcal{B}(\mathcal{H})$ (see Prop. 2.5) 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) $\widehat{u}^*\widehat{\pi}\;\widehat{u} = \Pi_{\rm r} + \mathcal{O}_{-\infty}(\varepsilon^\infty)$.

As a first step we modify $\widehat{u}$ by an $\mathcal{O}_0(\varepsilon^\infty)$-term in order to get a true unitary operator $\widetilde{U} \in \mathcal{U}(\mathcal{H})$ (which, in general, does not correspond to the Weyl quantization of any semiclassical symbol). Let

$$\widetilde{U} = (\widehat{u}^*\widehat{u})^{-\frac{1}{2}}\,\widehat{u}\,. \tag{30}$$

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 $\mathcal{O}_0(\varepsilon^\infty)$-close to the identity operator. Hence (30) defines a unitary operator which moreover is $\mathcal{O}_0(\varepsilon^\infty)$-close to $\widehat{u}$.

Finally we modify $\widetilde{U}$ in order to obtain a unitary which exactly intertwines $\Pi_{\rm r}$ and Π. Since $\|\widetilde{U}^*\Pi\,\widetilde{U} - \Pi_{\rm r}\| < 1$ for ε sufficiently small, the Nagy formula

$$W := \left[1 - \left(\widetilde{U}^*\Pi\,\widetilde{U} - \Pi_{\rm r}\right)^2\right]^{-\frac{1}{2}} \left[\widetilde{U}^*\Pi\,\widetilde{U}\,\Pi_{\rm r} + (1 - \widetilde{U}^*\Pi\,\widetilde{U})(1-\Pi_{\rm r})\right]$$

defines a unitary operator $W \in \mathcal{U}(\mathcal{H})$ such that $W^*\,\widetilde{U}^*\Pi\,\widetilde{U}\,W = \Pi_{\rm r}$ and $W = \mathbf{1} + \mathcal{O}_0(\varepsilon^\infty)$. Thus by defining $U = \widetilde{U}\,W$ one obtains (27), with the desired properties. □

Remark 4.4 We sketch how to prove the existence of a smooth map u_0 satisfying (26). Given

$$E = \left\{(z,\psi) \in \mathbb{R}^{2d} \times \mathcal{H}_{\rm f} : \psi \in \mathrm{Ran}\pi_0(z)\right\}$$

the map $\Pi_E : E \to \mathbb{R}^{2d}$, $(z,\psi) \mapsto z$ 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

$$w(z) = \left[1 - (\pi_0(z) - \pi_0(z_0))^2\right]^{-\frac{1}{2}} \left[\pi_0(z)\pi_0(z_0) + (1-\pi_0(z))(1-\pi_0(z_0))\right]$$

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

$$\begin{array}{rccccc} \Theta : & \Pi_E^{-1}(\mathcal{U}_{z_0}) & \to & \mathcal{U}_{z_0} \times \mathrm{Ran}\pi(z_0) & \to & \mathcal{U}_{z_0} \times \mathcal{K}_{\rm f} \\ & (z,\psi) & \mapsto & (z, w(z)\psi) & \mapsto & (z, \phi(z_0)w(z)\psi) \end{array}$$

where we use the fact that there exists a unitary operator $\phi(z_0) : \mathrm{Ran}\pi(z_0) \to \mathcal{K}_{\rm f}$. The existence of $\phi(z_0)$ follows from the fact that the dimension of $\mathrm{Ran}\pi(z_0)$ 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 $\mathcal{U}(\mathcal{K}_{\rm f})$-compatible, and the previous data define a linear $\mathcal{U}(\mathcal{K}_{\rm f})$-bundle.

Since the base space is contractible, the bundle is trivial and the associated principal $\mathcal{U}(\mathcal{K}_{\rm f})$-bundle (i.e. the bundle of the orthonormal frames) admits a global *smooth* section. This implies the existence of a *smooth* map $u_0 : \mathbb{R}^{2d} \to \mathcal{U}(\mathcal{H}_{\rm f})$ such that (26) holds true.

5 Adiabatic perturbation theory

5.1 The effective Hamiltonian

In the previous section we constructed a unitary U on $\mathcal{H}$ which exactly intertwines the almost invariant subspace RanΠ and the reference subspace $\mathcal{K} = \mathrm{Ran}\Pi_{\mathrm{r}}$. U and Π are $\mathcal{O}_0(\varepsilon^\infty)$-close to pseudodifferential operators with symbols u and π both in $S^0_\rho(\varepsilon)$.

We define the *effective Hamiltonian* $\widehat{h}$ as the quantization of a resummation h of the formal symbol

$$h = u^* \# H \# u\,. \tag{31}$$

Recall that we do not distinguish semiclassical symbols and formal symbols in the notation. 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 5.1 *Under the assumptions of Theorem 4.1, one has that $h \in S^m_\rho(\varepsilon)$ and $\widehat{h}$ is essentially self-adjoint on $\mathcal{S}$. Furthermore*

$$[\,\widehat{h},\, \Pi_{\mathrm{r}}\,] = 0\,, \tag{32}$$

$$e^{-i\widehat{H}t} - \widehat{u}\, e^{-i\widehat{h}t}\, \widehat{u}^* = \mathcal{O}_0(\varepsilon^\infty |t|) \tag{33}$$

and

$$e^{-i\widehat{H}t} - U\, e^{-i\widehat{h}t}\, U^* = \mathcal{O}_0(\varepsilon^\infty (1+|t|))\,. \tag{34}$$

Proof. Since $u \in S^0_\rho(\varepsilon)$ and $H \in S^m_\rho(\varepsilon)$, the composition rule for semiclassical operators (see Prop. 2.6) yields $h \in S^m_\rho(\varepsilon)$ and thus $h_j \in S^{m-j\rho}_\rho$.

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 $\mathcal{B}(\mathcal{H}_{\mathrm{f}})$-valued symbols, $\widehat{u}^{-1} \in OPS^0(\varepsilon)$ and thus $\widehat{u}^{-1}\mathcal{S} = \mathcal{S}$. Hence $\mathcal{S}$ is a core for $\widetilde{h}$ and, since $\widehat{h} - \widetilde{h} \in \mathcal{B}(\mathcal{H})$, the same conclusions hold for $\widehat{h}$.

Next observe that, by construction, $[h_j, \pi_{\mathrm{r}}] = 0$ for all $j \in \mathbb{N}$ and thus $[h_j, \pi_{\mathrm{r}}]_{\widetilde{\#}} = 0$ because π_{r} does not depend on $(q,p) \in \mathbb{R}^{2d}$. Hence $[\widehat{h}_j, \Pi_{\mathrm{r}}] = 0$ and thus (32) follows.

For (33) observe that

$$e^{-i\widehat{H}t} - \widehat{u}\, e^{-i\widehat{h}t}\, \widehat{u}^* = -\,i\, e^{-i\widehat{H}t} \int_0^t ds\, e^{i\widehat{H}s} \left(\widehat{H}\,\widehat{u} - \widehat{u}\,\widehat{h}\right) e^{-i\widehat{h}s}\, \widehat{u}^* = \mathcal{O}_0(\varepsilon^\infty |t|)\,,$$

since, by construction, $(\widehat{H}\,\widehat{u} - \widehat{u}\,\widehat{h}) = \mathcal{O}_{-\infty}(\varepsilon^\infty)$. Finally (34) follows from (33) using $U - \widehat{u} = \mathcal{O}_0(\varepsilon^\infty)$. □

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 (32), we can, whenever appropriate, restrict our attention to the reduced Hilbert space $\mathcal{K} = \mathrm{Ran}\Pi_{\mathrm{r}}$. 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 as $\| U - \widehat{u}^{(n)} \|_{\mathcal{B}(\mathcal{H})} = \mathcal{O}(\varepsilon^{n+1})$.

Our main interest are approximations to the solution of the time-dependent Schrödinger equation

$$i \, \frac{\partial \psi_t}{\partial t} = \widehat{H} \, \psi_t$$

over times of order $\varepsilon^{-k}\tau$, where τ does not depend on ε and $k \in \mathbb{N}$ is arbitrary. Starting with (33) on the almost invariant subspace we obtain

$$\begin{aligned} e^{-i\widehat{H}t}\Pi &= \widehat{u}\, e^{-i\widehat{h}t}\, \Pi_{\mathrm{r}}\, \widehat{u}^* + \mathcal{O}_0(\varepsilon^\infty |t|) \\ &= \widehat{u}^{(n)}\, e^{-it\widehat{h}^{(n+k)}}\, \Pi_{\mathrm{r}}\, \widehat{u}^{(n)*} + (1+|\tau|)\mathcal{O}_0(\varepsilon^{n+1}) \,, \quad |t| \leq \varepsilon^{-k}\tau \,, \end{aligned} \tag{35}$$

where $n + k \geq m - 1$ is assumed in order to have $\widehat{h} - \widehat{h}^{(n+k)} \in \mathcal{B}(\mathcal{H})$. 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 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 (35) to $n = 0$ and $k = 1$, one obtains the leading order solution of the Schrödinger equation as

$$e^{-i\widehat{H}t}\Pi = \widehat{u}_0\, e^{-i(\widehat{h}_0 + \varepsilon \widehat{h}_1)t}\, \Pi_{\mathrm{r}}\, \widehat{u}_0^* + (1+|\tau|)\mathcal{O}_0(\varepsilon) \,, \quad |t| \leq \varepsilon^{-1}\tau \,, \tag{36}$$

where $m \leq 2$. Here the choice of $k = 1$ corresponds to the macroscopic or semiclassical time-scale t/ε. On this time-scale the effective dynamics $e^{-i\widehat{h}t/\varepsilon}\Pi_{\mathrm{r}}$ on the reference subspace is expected to have a nice semiclassical limit, under suitable conditions on $\widehat{h}$.

Note that one can replace in (35) and analogously in (36) τ by $\varepsilon^{-\delta}\tau$ and obtains

$$e^{-i\widehat{H}t}\Pi = \widehat{u}^{(n)}\, e^{-i\widehat{h}^{(n+k)}}\, \Pi_{\mathrm{r}}\, \widehat{u}^{(n)*} + (1+|\tau|)\mathcal{O}_0(\varepsilon^{n+1-\delta}) \,, \quad |t| \leq \varepsilon^{-(k+\delta)}\tau \,. \tag{37}$$

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.

We emphasize that (35) and (36) 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 $e^{-i\widehat{H}t/\varepsilon}$ 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 7. On the other hand, a semiclassical expansion of the right hand side of (36) is straightforward in many interesting cases, as will be discussed in Section 6.

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 $E^{(n)}$ with an eigenfunction $o(\varepsilon^n)$-close to $U\psi^{(n)}$. 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 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$_1$, KMSW] yield in some respects mathematically stronger results. However, our scheme suffices for estimating asymptotic expansions of eigenvalues and is simpler to handle, in general.

5.2 Leading order terms in the expansion of the effective Hamiltonian

We turn to the explicit determination of the leading order terms h_j in the expansion of $\widehat{h}$ using (31). 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 4. 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 (31). The double Moyal product becomes rather awkward to handle, and alternatively we proceed inductively by observing that

$$H\,\#\,u - u\,\#\,h_0 = \varepsilon\,u\,\#\,h_1 + \mathcal{O}(\varepsilon^2) = \varepsilon\,u_0\,h_1 + \mathcal{O}(\varepsilon^2)\,, \tag{38}$$

with the subprincipal symbol on the left hand side being

$$\left(H\,\#\,u - u\,\#\,h_0\right)_1 = H_0u_1 + H_1u_0 - u_1h_0 + (H_0\,\#\,u_0)_1 - (u_0\,\#\,h_0)_1\,. \tag{39}$$

Recall the notation $a\,\#\,b = \sum_{j=0}^{\infty} \varepsilon^j\,(a\,\#\,b)_j$ for the expansion of the Moyal product, cf. Section 2. Combining (38) and (39) one obtains

$$h_1 = u_0^*\left(H_0u_1 + H_1u_0 - u_1h_0 + (H_0\,\#\,u_0)_1 - (u_0\,\#\,h_0)_1\,\right). \tag{40}$$

The expression (40) further simplifies if one specializes to the case where $\sigma_{\rm r}(q,p) = \{E_{\rm r}(q,p)\}$ consists of a single eigenvalue of $H_0(q,p)$ and one projects on the relevant subspace,

$$\pi_{\rm r} h_1 \pi_{\rm r} = \pi_{\rm r}\Big(u_0^*\, H_1\, u_0 + u_0^*(H_0 \,\#\, u_0)_1 - u_0^*(u_0 \,\#\, E_{\rm r})_1\Big)\pi_{\rm r}\,. \tag{41}$$

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 $\sigma_{\rm r}(q,p)$, one computes

$$\begin{aligned}\pi_{\rm r} h_2 \pi_{\rm r} \;=\; & \pi_{\rm r} u_0^*\Big(H_2 u_0 + H_1 u_1 - u_1 h_1 \\ & + (H_0 \,\#\, u_1)_1 + (H_1 \,\#\, u_0)_1 - (u_1 \,\#\, E_{\rm r})_1 - (u_0 \,\#\, h_1)_1 \\ & + (H_0 \,\#\, u_0)_2 - (u_0 \,\#\, E_{\rm r})_2\Big)\pi_{\rm r}\,.\end{aligned} \tag{42}$$

Again, (42) 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 4.

Although (42) 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 (42) 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 and 4 yields

$$u_1 = u_0\Big(-\frac{i}{4}\{u_0^*, u_0\} + [u_0^*\, \pi_1^{\rm OD}\, u_0, \pi_{\rm r}] + \frac{i}{4}[(\{u_0^*, \pi_0\}u_0 + u_0^*\{\pi_0, u_0\}), \pi_{\rm r}]\Big)\,, \tag{43}$$

with

$$\pi_1^{\rm OD} := \pi_0 \pi_1 (1-\pi_0) + (1-\pi_0)\pi_1\pi_0\,,$$

where we used that $(a \,\#\, b)_1 = -\frac{i}{2}\{a, b\}$. Recall the definition (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. One finds

$$\pi_1^{\rm OD} = \frac{i}{2}\left(R_0(E_{\rm r})(1-\pi_0)\{H_0 + E_{\rm r}, \pi_0\}\pi_0 + \pi_0\{\pi_0, H_0 + E_{\rm r}\}R_0(E_{\rm r})(1-\pi_0)\right)\,,$$

where $R_0(E_{\rm r})(1-\pi_0) = (H_0 - E_{\rm r})^{-1}(1-\pi_0)$ is uniformly bounded because of the gap condition. For sake of completeness we mention that $\pi_1 = \pi_1^{\rm OD} + \frac{i}{2}\{\pi_0, \pi_0\}$ 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 $E_{\rm r}(q,p)$, h_n depends only on $u^{(n-1)}$, $H^{(n)}$ and $h^{(n-1)}$ and is thus considerably easier to obtain.

Remark 5.2 Note that in the case of $\sigma_{\rm r}(q,p) = \{E_{\rm r}(q,p)\}$, the principal symbol $h_0(q,p) = E_{\rm r}(q,p)\mathbf{1}_{\mathcal{H}_{\rm f}}$ and the subprincipal symbol $h_1(q,p)$ as given by (41) are well defined regardless of the gap condition, provided that the spectral projection $\pi_0(q,p)$ is sufficiently regular. Indeed, it can be shown, at least in some special cases, that there is still adiabatic decoupling to leading order and an effective dynamics generated by $\widehat{h}_0 + \varepsilon\,\widehat{h}_1$ without a gap condition [Te$_1$], [Te$_2$].

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 suitable basis $\{\psi_\alpha(q,p)\}_{\alpha\in I}$ of $\mathrm{Ran}\pi_0(q,p)$ and defines $u_0(q,p) = \sum_{\alpha\in I} |\psi_\alpha(q,p)\rangle\langle\chi_\alpha| + r(q,p)$, where the vectors χ_α form a basis for $\mathrm{Ran}\pi_\mathrm{r}$ and $r(q,p)$ is some arbitrary unitary intertwining $\mathrm{Ran}\pi_\mathrm{r}^\perp$ and $\mathrm{Ran}\pi_0(q,p)^\perp$. $\pi_\mathrm{r}\, h_j(q,p)\,\pi_\mathrm{r}$ is independent of the choice of the unitary $r(q,p)$ for all $j\in\mathbb{N}$.

We remark 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 4.4). 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 $\sigma_\mathrm{r}(q,p) = \{E_\mathrm{r}(q,p)\}$ 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

$$h^{(1)}_{\alpha\beta} = \langle\chi_\alpha, h^{(1)}\chi_\beta\rangle = E_\mathrm{r}\,\delta_{\alpha\beta} + \varepsilon\, h_{1\,\alpha\beta}\,, \tag{44}$$

with

$$\begin{aligned} h_{1\,\alpha\beta} &= \langle\chi_\alpha, h_1\chi_\beta\rangle = \langle\psi_\alpha, H_1\psi_\beta\rangle - \frac{i}{2}\langle\psi_\alpha, \{(H_0+E_\mathrm{r}),\psi_\beta\}\rangle \\ &= \langle\psi_\alpha, H_1\psi_\beta\rangle - i\langle\psi_\alpha,\{E_\mathrm{r},\psi_\beta\}\rangle - \frac{i}{2}\langle\psi_\alpha, \{(H_0-E_\mathrm{r}),\psi_\beta\}\rangle\,. \end{aligned} \tag{45}$$

The indices α and β are matrix-indices, both running from 1 to ℓ. Equations (44) and (45) 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 (44) 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 7, for the Dirac equation h_1 governs the spin precession. The reason for the particular splitting of the terms in (45) will be discussed in Section 6. Here we only remark that the second term in (45) 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.

5.3 Born-Oppenheimer type Hamiltonians

An instructive example to which formula (45) applies are Born-Oppenheimer type Hamiltonians of the form

$$H_\mathrm{BO}(q,p) = \frac{1}{2}p^2\mathbf{1}_{\mathcal{H}_\mathrm{f}} + V(q)\,, \tag{46}$$

$V\in S^0(\mathcal{B}(\mathcal{H}_\mathrm{f}))$, with an electronic energy band $e_\mathrm{r}(q)$ of constant multiplicity ℓ, i.e. $V(q)\pi_0(q) = e_\mathrm{r}(q)\pi_0(q)$. Adiabatic decoupling for Born-Oppenheimer type Hamiltonians is established with exponentially small errors by Martinez and Sordoni [MaSo], see also [So]. Their result partly triggered our interest to develop a general theory.

Note that the quadratic growth of $H_\mathrm{BO}(q,p)$ as a function of p prevents from applying the general results directly. As to be discussed in Section 5.5, energy cutoffs need to be introduced. For the moment we ignore this problem and proceed by working out the perturbative scheme 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 $H_{\mathrm{BO}}(q,p)\psi_\alpha(q) = E_{\mathrm{r}}(q,p)\psi_\alpha(q)$ with $E_{\mathrm{r}}(q,p) = \frac{1}{2}p^2 + e_{\mathrm{r}}(q)$ for $1 \leq \alpha \leq \ell$. Only the second term of our formula (45) contributes and yields

$$h_{1\,\alpha\beta}(q,p) = -i\,p\cdot\langle\psi_\alpha(q), \nabla_q\psi_\beta(q)\rangle =: -\,p\cdot A_{\alpha\beta}(q)\,,$$

which is well known in the case of a nondegenerate eigenvalue, [ShWi, LiWe, TeSp]. $A_{\alpha\beta}(q)$ 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 so called Berry connection. As mentioned already, a more detailed discussion of the origin of the Berry connection will be given in Section 6.

For the Born-Oppenheimer Hamiltonian the calculation of $h_{2\,\alpha\beta}$ is still feasible without much effort and the result is

$$h_{2\,\alpha\beta} = \frac{1}{2}\sum_{\mu=1}^{\ell} A_{\alpha\mu}\cdot A_{\mu\beta} + \frac{1}{2}\langle\nabla_q\psi_\alpha, \cdot\nabla_q\psi_\beta\rangle - \langle\, p\cdot\nabla_q\psi_\alpha,\, R_0(E_{\mathrm{r}})\; p\cdot\nabla_q\psi_\beta\rangle\,. \qquad (47)$$

Recall the definition of $R_0(E_{\mathrm{r}}) = (H_0 - E_{\mathrm{r}})^{-1}(1-\pi_0)$, which reduces to $R_0(E_{\mathrm{r}})(q) = (V(q)-e_{\mathrm{r}}(q))^{-1}(1-\pi_0(q))$ in the present case. Although we omit the details of the computation leading to (47), we shortly describe how (42) relates to (47). Since $H_1 = 0$ and $H_2 = 0$ the corresponding terms in (42) do not contribute. Since u_0 and π_0 are functions of q only, the second term in (43) is the only one contributing to u_1, and thus the third term in (42) also vanishes after projecting with the π_{r}'s from outside the brackets. The last two terms in (42) cancel each other. The seventh term in (42) yields the first term in (47) and the fourth and sixth term in (42) combine to the second and third term in (47). In particular the calculation yields for the symbol of the unitary

$$u_{\mathrm{BO}}(q,p)\pi_{\mathrm{r}} = \sum_{\alpha=1}^{\ell}\Big(|\psi_\alpha(q)\rangle + i\varepsilon\, R_0(E_{\mathrm{r}})(q)\;|\,p\cdot\nabla_q\psi_\alpha(q)\rangle\Big)\langle\chi_\alpha| + \mathcal{O}(\varepsilon^2)\,.$$

Thus the symbol of the second order effective Born-Oppenheimer Hamiltonian reads

$$\begin{aligned} h_{\mathrm{BO}\,\alpha\beta}(q,p) \;&=\; \frac{1}{2}\Big(p-\varepsilon\,A(q)\Big)^2_{\alpha\beta} + \,e_{\mathrm{r}}(q)\delta_{\alpha\beta} + \frac{\varepsilon^2}{2}\langle\nabla_q\psi_\alpha(q), \cdot\nabla_q\psi_\beta(q)\rangle \\ &\quad -\varepsilon^2\,\langle\, p\cdot\nabla_q\psi_\alpha(q),\, R_0(E_{\mathrm{r}})(q)\; p\cdot\nabla_q\psi_\beta(q)\rangle + \mathcal{O}(\varepsilon^3)\,, \end{aligned} \qquad (48)$$

where the first term from (47) nicely completes the square to the first term in (48). Note that the third term on the right side of (48) depends on q only and was interpreted in [ShWi] as a geometric electric potential in analogy to the geometric vector potential $A(q)$.

In the special case of a nondegenerate eigenvalue e_{r} and a matrix-valued Hamiltonian H, (48) reduces to the expression obtained by Littlejohn and Weigert [LiWe]. They also remark that the previous studies [ShWi, AhSt] of the expansion of the effective Born-Oppenheimer Hamiltonian missed the last term in (48). This strengthens our point of the usefulness of a general and systematic space-adiabatic perturbation theory.

The full power of our scheme is in force in cases where $\mathrm{Ran}\pi_0$ is degenerate and depends both on q and p, since then the known techniques [LiFl, LiWe, NeSo, MaSo] cannot be applied. The simplest example of this kind is the one-particle Dirac equation with slowly varying electric and magnetic potentials, which will be discussed in Section 7.

5.4 The time-adiabatic theory revisited

With little additional effort our scheme can be applied even to the time-adiabatic setup. As for notation, 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. Given a Hilbert space $\mathcal{H}$ and family $H^\varepsilon(t)$, $t \in \mathbb{R}$ of self-adjoint operators such that $H^\varepsilon(t) =: H(t,\eta,\varepsilon) \in S^0(\varepsilon, \mathcal{B}(\mathcal{H}))$, the solutions of the equations

$$i\varepsilon\partial_t U^\varepsilon(t,s) = H^\varepsilon(t) U^\varepsilon(t,s)\,, \qquad s \in \mathbb{R}\,, \tag{49}$$

define a *unitary propagator.* A unitary propagator is a unitary operator-valued map $U(t,s)$ strongly continuous in t and s jointly, such that

$$U(t,t) = \mathbf{1}_\mathcal{H} \qquad \text{and} \qquad U(t,r)U(r,s) = U(t,s)$$

for any $r,s,t \in \mathbb{R}$. In particular we have that $U^\varepsilon(t,0)\psi_0$ solves the time-dependent Schrödinger equation (2) for any $\psi_0 \in \mathcal{H}$.

It is assumed in addition that $H_0(t)$, the principal symbol of $H^\varepsilon(t)$, has a relevant part $\sigma_\mathrm{r}(t)$ 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 $\sigma_\mathrm{r}(t)$ by $\pi_0(t)$.

The following theorem is a variant of the *time-adiabatic theorem of quantum mechanics* [Ka$_1$, ASY, JoPf, Ne$_1$], however formulated in the language of adiabatic perturbation theory. Sjöstrand first recognized the usefulness of pseudodifferential calculus in this context [Sj] and we are grateful to G. Nenciu for pointing this out to us. We remark that 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 Pauli-Fierz Hamiltonian with *slowly* varying time-dependent external potentials.

Theorem 5.3 (Time-adiabatic theorem) *Let $H(t)$ and $\sigma_\mathrm{r}(t)$ be as above.*

(i) Decoupled subspace. *There exists a family of orthogonal projectors $\Pi(t)$ such that $\Pi(\cdot) \in S^0(\varepsilon, \mathcal{B}(\mathcal{H}))$, $\Pi(t) - \pi_0(t) = \mathcal{O}_0(\varepsilon)$ and*

$$U(t,s)^*\,\Pi(t)\,U(t,s) = \Pi(s) + \mathcal{O}_0(\varepsilon^\infty|t-s|) \tag{50}$$

uniformly for $s,t \in \mathbb{R}$. Whenever $\partial_t^\alpha H(t) = 0$ for some $t \in \mathbb{R}$ and all $\alpha \in \mathbb{N}$, then $\Pi(t) = \pi_0(t)$.

(ii) Intertwining unitaries. *There exists a family of unitaries $u_0(\cdot) \in C^\infty_\mathrm{b}(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ with $u_0^*(t)\,\pi_0(t)\,u_0(t) = \pi_0(0) =: \pi_\mathrm{r}$ and a family of unitaries $\mathcal{U}(\cdot) \in S^0(\varepsilon, \mathcal{B}(\mathcal{H}))$ such that*

$$\mathcal{U}^*(t)\,\Pi(t)\,\mathcal{U}(t) = \pi_\mathrm{r} \quad \textit{and} \quad \mathcal{U}(t) - u_0(t) = \mathcal{O}_0(\varepsilon)\,.$$

(iii) Effective dynamics. *There exists a family of self-adjoint operators $h(t)$, $h(\cdot) \in S^0(\varepsilon, \mathcal{B}(\mathcal{H}))$, such that*

$$[\,h(t),\,\pi_\mathrm{r}\,] = 0 \qquad \textit{for all} \qquad t \in \mathbb{R} \tag{51}$$

and the solution of the initial value problem

$$i\varepsilon\partial_t U_\mathrm{eff}(t,s) = h(t) U_\mathrm{eff}(t,s)\,, \qquad s \in \mathbb{R}\,, \qquad U_\mathrm{eff}(t,t) = \mathbf{1}_\mathcal{H}$$

satisfies

$$U(t,s) = \mathcal{U}(t)\, U_{\rm eff}(t,s)\, \mathcal{U}^*(s) + \mathcal{O}_0(\varepsilon^\infty |t-s|)\,. \tag{52}$$

The asymptotic expansion of $h(t)$ in $\mathcal{B}(\mathcal{H})$ reads

$$h(t) \asymp \sum_{n=0}^{\infty} \varepsilon^n \left(\sum_{j+k+l=n} u_j^*(t)\, H_k(t)\, u_l(t) + \frac{i}{2} \sum_{j+k+1=n} \left(u_j^*(t)\, \dot u_k(t) - \dot u_j^*(t)\, u_k(t) \right) \right), \tag{53}$$

where $\sum_n \varepsilon^n H_n(t)$ is the asymptotic expansion of $H(t)$ in $\mathcal{B}(\mathcal{H})$ and $\sum_n \varepsilon^n u_n$ is the asymptotic expansion of $\mathcal{U}(t)$ in $\mathcal{B}(\mathcal{H})$.

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 ${\rm Ran}\pi_0(t)$, the effective Hamiltonian including second order reads

$$h_{\alpha\beta}(t) = e_{\rm r}(t)\delta_{\alpha\beta} \;-\; i\,\varepsilon\, \langle \varphi_\alpha(t), \dot\varphi_\beta(t)\rangle \;+\; \frac{\varepsilon^2}{2} \langle \dot\varphi_\alpha(t), R_0(e_{\rm r})\, \dot\varphi_\beta(t)\rangle \;+\; \mathcal{O}(\varepsilon^3)\,,$$

where $R_0(e_{\rm r}) = (H(t) - e_{\rm r}(t))^{-1}\,(1-\pi_0(t))$. For the unitary $\mathcal{U}(t)$ one finds

$$\mathcal{U}(t)\pi_{\rm r} = \sum_{\alpha=1}^{\ell} \Big(|\varphi_\alpha(t)\rangle + i\varepsilon\, R_0(e_{\rm r})(t)\;|\dot\varphi_\alpha(t)\rangle \Big) \langle \varphi_\alpha(0)| + \mathcal{O}(\varepsilon^2)\,.$$

Proof. In order to apply the general scheme developed in the previous sections it is convenient – in analogy with the extended configuration space in classical mechanics – to introduce the extended space $\mathcal{K} = L^2(\mathbb{R}, \mathcal{H}) = \int_{\mathbb{R}}^{\oplus} \mathcal{H}\; dt$ and to define the extended Hamiltonian

$$\widehat{K} = -i\varepsilon \partial_t + H(t)$$

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 $e^{-i\widehat K \sigma}$, $\sigma \in \mathbb{R}$, is related to the unitary propagator (49) through

$$\left(e^{-i\widehat K\sigma} \psi \right)(t) = U(t, t-\sigma)\psi(t-\sigma)\,. \tag{54}$$

Moreover, the unitary group $e^{-i\widehat K\sigma}$ 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 $S^1_1(\mathcal{B}(\mathcal{H}))$.

By assumption $K \in S^1_1$ satisfies assumption $({\rm Gap})_\sigma$ with $\sigma = 0$. However, because of the simple dependence of $K(t,\eta)$ on η, the conclusion of Theorem 3.1 and 4.1 hold still true in a sense to be made precise.
Indeed, by following the proof of Lemma 3.2 one gets a semiclassical symbol $\pi \in S^0_0(\varepsilon, \mathcal{B}(\mathcal{H}))$, depending on t only, such that $[K,\pi]_{\tilde\#} \asymp 0$ in $S^1_0(\varepsilon)$. On the other hand,

$$[K,\pi]_{\tilde\#} = [H,\pi]_{\tilde\#} + [\eta,\pi]_{\tilde\#} = [H,\pi]_{\tilde\#} - i\varepsilon\,(\partial_t\pi)$$

where the last equality follows from the fact that $[\eta,\pi]_{\tilde\#}$ is the Weyl symbol of $[-i\varepsilon\partial_t, \pi(t)] = -i\varepsilon\,(\partial_t\pi)\,(t)$. Since both $[H,\pi]_{\tilde\#}$ and $\partial_t\pi$ belong to $S^0_0(\varepsilon)$, one concludes that the asymptotic expansion $[K,\pi]_{\tilde\#} \asymp 0$ holds true in $S^0_0(\varepsilon)$, and hence $[\widehat K, \widehat\pi] = \mathcal{O}_0(\varepsilon^\infty)$. Finally one defines

$$\Pi(t) = \frac{i}{2\pi} \int_{|\zeta - 1| = \frac12} (\pi(t) - \zeta)^{-1} d\zeta$$

and finds $\Pi(\cdot) \in S^0(\varepsilon, \mathcal{B}(\mathcal{H}))$, $\Pi(t) - \pi(t) = \mathcal{O}_0(\varepsilon^\infty)$ and $[e^{-i\widehat{K}\sigma}, \Pi] = \mathcal{O}_0(\varepsilon^\infty|\sigma|)$ as in Section 3. Together with (54) this implies

$$\operatorname*{ess\,sup}_{t\in\mathbb{R}} \|U(t, t-\sigma)^* \, \Pi(t) \, U(t, t-\sigma) - \Pi(t-\sigma)\|_{\mathcal{B}(\mathcal{H})} = \mathcal{O}_0(\varepsilon^\infty|\sigma|) \, .$$

However, since $\Pi(t)$ and $U(t,s)$ are continuous functions of t, the pointwise statement (50) follows.

As for the construction of $u_0(t)$, note that local versions of $u_0(t)$ clearly exist and that it is possible to glue them together in such a way to obtain a global version $u_0 \in C_\mathrm{b}^\infty$. $\mathcal{U}$ can be obtained as in Section 4, 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 $\mathcal{U}(t)$.

As in the general setting let the effective Hamiltonian be defined as a resummation of

$$k(\eta, t, \varepsilon) = (u^* \# K \# u)(\eta, t, \varepsilon) =: \eta + h(t, \varepsilon) \, ,$$

with the explicit expansion (53). According to Theorem 5.1 we then have

$$e^{-i\widehat{K}\sigma} - \mathcal{U} \, e^{-i\widehat{k}\sigma} \, \mathcal{U}^* = \mathcal{O}(\varepsilon^\infty|\sigma|) \, ,$$

which implies according to (54) that

$$\operatorname*{ess\,sup}_{t\in\mathbb{R}} \|U(t, t-\sigma) - \mathcal{U}(t) \, U_{\mathrm{eff}}(t, t-\sigma) \, \mathcal{U}^*(t-\sigma)\|_{\mathcal{B}(\mathcal{H})} = \mathcal{O}_0(\varepsilon^\infty|\sigma|) \, .$$

The pointwise statement (52) follows again from the continuous dependence on t of all involved expressions. □

5.5 Energy cutoff

The Born-Oppenheimer type Hamiltonians as well as many other physically relevant Hamiltonians do not satisfy the general assumptions we imposed in Sections 3 and 4. 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. 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. 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 [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 (46), 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 basically 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 (46) satisfies $H_0 \in S^2_0$ and it is elliptic provided that V is positive (otherwise just add a constant to H_0 since $V \in S^0$). Then we can prove adiabatic decoupling uniformly for energies below any $\lambda \in \mathbb{R}$, i.e. on $\mathrm{Ran}\,1\!\!1_{(-\infty,\lambda]}(\widehat{H}_0)$.

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 $\chi_\lambda \in C_0^\infty(\mathbb{R})$ such that $\chi_\lambda|_{[0,\lambda]} = 1$ and $\chi_\lambda|_{[\lambda+\delta,\infty)} = 0$ for some $\delta > 0$, then $\chi_\lambda(\widehat{H}_0) \in \mathrm{OP}S_0^{-\infty}$ is a semiclassical operator. Furthermore, its symbol $\chi := \mathrm{Symb}(\chi_\lambda(\widehat{H}_0))$ 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 developped e.g. in [DiSj], Theorem 8.7.

Next we assume that one can define an auxiliary Hamiltonian $H_{\mathrm{aux}}(q,p) \in S^0_0$ such that

(i) $H_{\mathrm{aux}}(q,p) = H_0(q,p)$ for all $(q,p) \in \Lambda + \delta := \{(q,p) : H_0(q,p) < \lambda + \delta\}$,

(ii) $H_{\mathrm{aux}}(q,p) > H_0(q',p')$ for all $(q,p) \notin \Lambda + \delta$ and $(q',p') \in \Lambda + \delta$

(iii) and $H_{\mathrm{aux}}(q,p)$ satisfies the global gap condition $(\mathrm{Gap})_0$.

This can be easily achieved e.g. in the Born-Oppenheimer setting by replacing p^2 by an appropriate bounded function.

It follows from the previous discussion that $(\,\widehat{H}_0 - \widehat{H}_{\mathrm{aux}}\,)\,\chi_\lambda(\widehat{H}_0) = \mathcal{O}_{-\infty}(\varepsilon^\infty)$ and that $\chi_\lambda(\widehat{H}_0) - \chi_\lambda(\widehat{H}_{\mathrm{aux}}) = \mathcal{O}_{-\infty}(\varepsilon^\infty)$. Using $\chi_\lambda(\widehat{H}_0)1\!\!1_{(-\infty,\lambda]}(\widehat{H}_0) = 1\!\!1_{(-\infty,\lambda]}(\widehat{H}_0)$, one finds, in particular, that

$$\left(\widehat{H}_0 - \widehat{H}_{\mathrm{aux}}\right)\,1\!\!1_{(-\infty,\lambda]}(\widehat{H}_0) = \mathcal{O}_0(\varepsilon^\infty) \tag{55}$$

in the norm of bounded operators and thus also

$$\begin{aligned} &\left(e^{-i\widehat{H}_{\mathrm{aux}}t} - e^{-i\widehat{H}_0 t}\right)1\!\!1_{(-\infty,\lambda]}(\widehat{H}_0) \qquad (56)\\ &= \;-\,ie^{-i\widehat{H}_{\mathrm{aux}}t}\int_0^t ds\, e^{i\widehat{H}_{\mathrm{aux}}s}\left(\widehat{H}_{\mathrm{aux}} - \widehat{H}_0\right)e^{-i\widehat{H}_0 s}\,1\!\!1_{(-\infty,\lambda]}(\widehat{H}_0) = \mathcal{O}_0(\varepsilon^\infty|t|)\,. \end{aligned}$$

Now the scheme of Sections 3, 4 and 5 can be applied to H_{aux} and by virtue of (55) and (56) 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 $h_{\mathrm{aux}} = U^*\widehat{H}_{\mathrm{aux}}U$ are given by the formulas obtained in Section 5.2 using the symbol $H_0(q,p)$.

6 Semiclassical analysis 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 and U, but no semiclassical limit has been performed. Indeed, the adiabatic decoupling of energy bands is a purely quantum phenomenon, which is, in general, independent from the semiclassical limit.

However, under the assumption that $\sigma_{\mathrm{r}}(q,p) = \{E_{\mathrm{r}}(q,p)\}$ 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. $h_0(q,p)\pi_{\mathrm{r}} = E_{\mathrm{r}}(q,p)\mathbf{1}_{\mathcal{K}_{\mathrm{f}}}$, and a semiclassical analysis of $\widehat{h}$ can be done in a standard way. In particular, the dynamics of quantum observables can be approximated by quantities constructed using only the classical flow Φ^t generated by the (classical, scalar) Hamiltonian $E_{\mathrm{r}}(q,p)$. This results in a generalized Egorov's theorem, see Theorem 6.1. We emphasize that for more general energy bands $\sigma_{\mathrm{r}}(q,p)$ one cannot expect a simple semiclassical limit, at least not in the usual sense.

6.1 Semiclassical analysis for matrix-valued symbols

Egorov's Theorem. 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 the Heisenberg equations of motion for semiclassical observables: Let $a(q,p,\varepsilon) \in S^0_1(\varepsilon, \mathcal{B}(\mathbb{C}^\ell))$, then the quantum mechanical time evolution of $\widehat{a}$ is given by

$$\widehat{a}(t) = e^{i\widehat{h}t/\varepsilon}\,\widehat{a}\,e^{-i\widehat{h}t/\varepsilon}$$

and satisfies

$$\frac{d\,\widehat{a}(t)}{dt} = \frac{i}{\varepsilon}[\,\widehat{h},\,\widehat{a}(t)]\,. \tag{57}$$

Expanding both sides of (57) 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:

$$\begin{aligned}
\frac{d\,a_0(t)}{dt} &= \{E_{\mathrm{r}}\mathbf{1}, a_0(t)\} + i[h_1, a_0(t)] && (58)\\
\frac{d\,a_1(t)}{dt} &= \{E_{\mathrm{r}}\mathbf{1}, a_1(t)\} + i[h_1, a_1(t)] - \frac{1}{2}(\{h_1, a_0(t)\} - \{a_0(t), h_1\}) \\
&\quad + i[h_2, a_0(t)] && (59)\\
\frac{d\,a_2(t)}{dt} &= \{E_{\mathrm{r}}\mathbf{1}, a_2(t)\} + i[h_1, a_2(t)] + \ldots\,. && (60)
\end{aligned}$$

Since $da_n(t)/dt$ does not depend on higher orders, the equations can be solved iteratively. The solution of (58) with initial condition $a_0(q,p,0) = a_0(q,p)$ is given through

$$a_0(q,p,t) = D^*(q,p,t)\,a_0(\Phi^t(q,p))\,D(q,p,t)\,, \tag{61}$$

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

$$\frac{\partial}{\partial t} D(q,p,t) = -\, i\, h_1(\Phi^t(q,p))\, D(q,p,t)\,. \tag{62}$$

with initial condition $D(q,p,0) = \mathbf{1}$. One can think of (62) 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 (62) is unitary for all $(q,p,t) \in \mathbb{R}^{2d} \times \mathbb{R}$.

To see that (61) is indeed the solution of (58), note that the mappings

$$\mathcal{U}(t) : C_\mathrm{b}(\mathbb{R}^{2d}, \mathcal{B}(\mathbb{C}^\ell)) \to C_\mathrm{b}(\mathbb{R}^{2d}, \mathcal{B}(\mathbb{C}^\ell))$$

defined through (61) for $t \in \mathbb{R}$, i.e.

$$(\mathcal{U}(t)\, a_0)(q,p) = D^*(q,p,t)\, a_0(\Phi^t(q,p))\, D(q,p,t)\,, \tag{63}$$

form a one-parameter group of linear automorphisms on the Banach space $C_\mathrm{b}(\mathbb{R}^{2d}, \mathcal{B}(\mathbb{C}^\ell))$, since

$$\begin{aligned}
(\mathcal{U}(s)\, \mathcal{U}(t)\, a_0)(q,p) &= D^*(q,p,s)\, D^*(\Phi^s(q,p),t)\, a_0(\Phi^s \circ \Phi^t(q,p))\, D(\Phi^s(q,p),t)\, D(q,p,s) \\
&= D^*(q,p,t+s)\, a_0(\Phi^{t+s}(q,p))\, D(q,p,t+s) \\
&= (\mathcal{U}(t+s) a_0)(q,p)\,.
\end{aligned}$$

Here the group structures of Φ^t and of the solutions of (62) are used. Hence $\mathcal{U}(t)$ is a group and it suffices to check that (61) solves (58) at time $t = 0$, which is easy to see.

The physical interpretation becomes simpler when translated to the states: a "classical" particle which started at time 0 at the phase space point (q,p) with spinor $\varphi_0 \in \mathbb{C}^\ell$, is at time t located at the phase space point $\Phi^t(q,p)$ with spinor $\varphi_t = D(q,p,t)\varphi_0$. Hence (62) implies that

$$\frac{d\varphi_t}{dt} = -\, i\, h_1(\Phi^t(q,p))\, \varphi_t\,. \tag{64}$$

One can also think of $\mathcal{U}(t)$ as being the action on observables of a "classical" flow Φ^t_ℓ on phase space $\mathbb{R}^{2d} \times \mathrm{SU}(\ell)$ defined as

$$\Phi^t_\ell(q,p,U) = (\Phi^t(q,p), D(q,p,t)\, U)\,.$$

Turning to the higher order corrections (59), (60) etc., they are of the form

$$\frac{d\, a_n(t)}{dt} = \{E_\mathrm{r}\mathbf{1}, a_n(t)\} + i[h_1, a_n(t)] + I_n(a_0(t), \dots, a_{n-1}(t))$$

with an inhomogeneity $I_n(t)$ depending only on the known functions $a_0(t), \dots, a_{n-1}(t)$. Thus, assuming $a_n(0) = 0$, one finds

$$a_n(t) = \int_0^t ds\, \mathcal{U}(t-s)\, I_n(s)\,. \tag{65}$$

In order to solve Equation (59) 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 (59) vanishes at all times, since, according to (61), $a_0(t)$ is a scalar multiple of the identity for all times. In Section 7 the back reaction of the spin of an electron on its translational motion will be discussed on the basis of (59).

We summarize the preceding discussion on Egorov's theorem.

Theorem 6.1 (Egorov) *Let H satisfy either (IG)$_m$ for $m \leq 1$ and $\rho = 1$ or (CG) with $\rho = 0$. Let $\sigma_{\rm r}(q,p) = \{E_{\rm r}(q,p)\}$ be an eigenvalue of $H_0(q,p)$ of finite multiplicity ℓ.*
Then the classical flow Φ^t generated by $E_{\rm r}(q,p)$ and the solution of (62) with initial condition $D(q,p,0) = \mathbf{1}$ exist globally in time. For $a_0 \in S^0_\rho(\mathcal{B}(\mathbb{C}^\ell))$, $a_0(t)$ given by (61) is a solution of (58) and $a_0(t) \in S^0_\rho(\mathcal{B}(\mathbb{C}^\ell))$ for all t.
For each $T < \infty$ there is a constant $C_T < \infty$ such that for all $t \in [-T,T]$

$$\|a(t) \,-\, \mathcal{W}_\varepsilon\,(a_0(t))\| \,\leq\, \varepsilon\, C_T\,, \tag{66}$$

where $a(t) = e^{i\widehat{h}t/\varepsilon}\,\widehat{a}_0\,e^{-i\widehat{h}t/\varepsilon}$.

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 (57) rigorous, note that $E_{\rm r} = \pi_{\rm r} h_0 \pi_{\rm r} \in S^m_\rho(\mathbb{R})$ 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 (61). Thus one can interchange quantization and differentiation with respect to time and obtains

$$\begin{aligned} a(t) - \mathcal{W}_\varepsilon(a_0(t)) \;&=\; \int_0^t ds\,\frac{d}{ds}\left(e^{i\widehat{h}s/\varepsilon}\,\mathcal{W}_\varepsilon(a_0(t-s))\,e^{-i\widehat{h}s/\varepsilon}\right) \\ &=\; \int_0^t ds\,e^{i\widehat{h}s/\varepsilon}\left(\frac{i}{\varepsilon}\left[\widehat{h},\mathcal{W}_\varepsilon(a_0(t-s))\right] - \mathcal{W}_\varepsilon\left(\frac{da_0}{dt}(t-s)\right)\right)e^{-i\widehat{h}s/\varepsilon}\,. \end{aligned}$$

Now, by construction, $\frac{i}{\varepsilon}\left[\widehat{h},\widehat{a_0(t-s)}\right] - \mathcal{W}_\varepsilon\left(\frac{da_0}{dt}(t-s)\right)$ 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 (66) follows. $\square$

This matrix-valued version of Egorov's theorem has been discussed several times in the literature [Iv, BrNo].

Berry connection. With this preparation we explain the motivation behind the particular splitting of the terms in (45). It is of geometrical origin and related to the Berry connection. Recall that in the Born-Oppenheimer setting $h_{1\,\alpha\beta}(q,p) = -p\cdot A_{\alpha\beta}(q)$ and thus $A_{\alpha\beta}(q)$ 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 trivial connection on the trivial bundle $\mathbb{R}^d \times \mathcal{H}_{\rm f}$ induces on the subbundle defined by $\pi_0(q)$. If one assumes that $\mathrm{Ran}\pi_0(q)$ 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, ShWi, Si].

In the general case the second term of $h_{1\,\alpha\beta}(q,p)$ in (45), which we denote by

$$h_{{\rm Be}\,\alpha\beta}(q,p) = -i\langle\psi_\alpha(q,p),\{E_{\rm r},\psi_\beta\}(q,p)\rangle,$$

corresponds exactly to this parallel transport along the generalized Berry connection. More precisely, the trivial connection on the trivial bundle $\mathbb{R}^{2d} \times \mathcal{H}_{\rm f}$ induces a $U(\ell)$-connection on the subbundle defined by $\pi_0(q,p)$. After unitary rotation $u_0(q,p)$ the coefficients of this connection on the bundle $\mathbb{R}^{2d} \times \mathbb{C}^\ell$ are

$$A_{\alpha\beta}(q,p) = \,i\,\left(\begin{array}{c}\langle\psi_\alpha(q,p),\nabla_q\psi_\beta(q,p)\rangle\\ \langle\psi_\alpha(q,p),\nabla_p\psi_\beta(q,p)\rangle\end{array}\right),$$

in the sense that a section $s(q,p)$ is parallel if $(\nabla - iA)s = 0$. It is parallel along some curve $c(\tau) = (q(\tau), p(\tau))$ in $\mathbb{R}^{2d}$ if

$$\Big(\partial_\tau - \dot c(\tau)\cdot iA(q(\tau),p(\tau))\Big) s(q(\tau),p(\tau)) = 0\,.$$

For classical trajectories, where $\dot c(t) = (\nabla_p E_{\rm r}, -\nabla_q E_{\rm r})^{\rm T}$, this condition becomes

$$\Big(\partial_t + i\, h_{\rm Be}(q(t),p(t))\Big) s(q(t),p(t)) = 0\,. \tag{67}$$

If $h_1 = h_{\rm Be}$, (67) is exactly Equation (64) for the rotation of the spinor $\varphi_t(q(t),p(t)) = D(q,p,t)\varphi_0$ along the trajectory of the particle. This means if $h_1 = h_{\rm Be}$, 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.

Wigner function approach. The previous results on the time-evolution of semiclassical observables translate, by the duality expressed through

$$\langle \psi,\, \widehat{a}_0\, \psi\rangle = \int_{\mathbb{R}^{2d}} {\rm Tr}_{\mathbb{C}^\ell}\, \big(a_0(q,p) W^\psi(q,p)\big)\; dq\, dp\,,$$

to the time-evolution of the Wigner transform

$$W^\psi(q,p) := {\rm Symb}(P_\psi)(q,p) = (2\pi)^{-d}\int_{\mathbb{R}^d} d\xi\, e^{i\xi\cdot p}\, \psi(q+\varepsilon\xi/2)\otimes\psi^*(q-\varepsilon\xi/2)$$

as

$$\langle \psi,\, \widehat{a}_0(t)\, \psi\rangle = \int_{\mathbb{R}^{2d}} {\rm Tr}_{\mathbb{C}^\ell}\, \big(a_0(q,p)\, D^*(q,p,-t)\, W^\psi(\Phi^{-t}(q,p))\, D(q,p,-t)\big)\; dq\, dp + \mathcal{O}(\varepsilon)\,.$$

Transport equations for matrix-valued Wigner measures were derived in [GMMP] and applied to the Dirac equation in [Sp].

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

$$(e^{-i\widehat{h}t/\varepsilon}\psi)(x) = \int_{\mathbb{R}^d} dy\, K^\varepsilon(x,y,t)\,\psi(y)\,. \tag{68}$$

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

$$K^\varepsilon(x,y,t) = \frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^d} dp\, e^{\frac{i}{\varepsilon}\left(S(x,p,t) - y\cdot p\right)}\Big(\sum_{j=0}^\infty \varepsilon^j a_j(x,p,t)\Big)\,,$$

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 (68) at time $t=0$, i.e. $K^\varepsilon(x,y,0)=\delta(x-y)$, imposes the following initial conditions on S and $\{a_j\}_{j\geq 0}$:

$$S(x,p,0)=x\cdot p\,,\qquad a_0(x,p,0)=\mathbf{1}\quad\text{and}\quad a_j(x,p,0)=0\quad\text{for}\, j\geq 1\,.$$

For later times the coefficients are determined by formally expanding the Schrödinger equation for $K^\varepsilon(x,y,t)$

$$i\,\varepsilon\frac{\partial}{\partial t}K^\varepsilon(\cdot,y,t)=\widehat{h}\,K^\varepsilon(\cdot,y,t)$$

in orders of ε. At leading order only $\widehat{h}_0=\widehat{E}_0$ contributes and one obtains as in the scalar case

$$\partial_t\,S(x,p,t)+E_\mathrm{r}(x,\nabla_x S(x,p,t))=0\,, \tag{69}$$

the Hamilton-Jacobi equation for the symbol h_0. The next to leading order equation is the so called transport equation for a_0:

$$i\partial_t a_0(x,p,t)=\mathcal{L}(x,p,t)\,a_0(x,p,t)\;+h_1(x,\nabla_x S(x,p,t))\,a_0(x,p,t)\,. \tag{70}$$

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 (58), also in (70) h_1 contributes as an additional rotation in the transport equation for the leading order term. Since the solution of (69) exists only until a caustic is reached, the approximation (69), (70) to the propagator is a short time result only. The extension to arbitrary times is a complicated task, in general [MaFe].

6.2 An Egorov theorem

Ultimately the goal is to approximate expectation values of observables in 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, LiWe, 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 $\mathcal{K}=\mathrm{Ran}\Pi_\mathrm{r}$ 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 $\widehat{p}_\mathcal{H}=-i\varepsilon\nabla_x\otimes\mathbf{1}_{\mathcal{H}_\mathrm{f}}$ 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 $\widehat{p}_\mathcal{K}=-i\varepsilon\nabla_x\otimes\mathbf{1}_{\mathcal{K}_\mathrm{f}}$ be the same operators acting on $\mathcal{K}$. Then $\widehat{q}_\mathcal{K}=\Pi_\mathrm{r}U^*\,\widehat{q}_\mathcal{H}\,U\,\Pi_\mathrm{r}+\mathcal{O}(\varepsilon)$ and $\widehat{p}_\mathcal{K}=\Pi_\mathrm{r}\,U^*\,\widehat{p}_\mathcal{H}\,U\,\Pi_\mathrm{r}+\mathcal{O}(\varepsilon)$, with a, in general, nonvanishing ε-correction. 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 $\widehat{q}_{\mathcal{K}} = \Pi_{\mathrm{r}} U^* \, \widehat{q}_{\mathcal{H}} \, U \, \Pi_{\mathrm{r}} + \mathcal{O}(\varepsilon^2)$.

With this warning we exploit that semiclassical observables do not change after unitary rotation in leading order and state the Egorov theorem for the observables in the original representation.

Corollary 6.2 *Let H satisfy either (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 $b_0 \in S^0_1(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ such that $[b_0, \pi_0] = 0$ and $B(t) := e^{i\widehat{H}t/\varepsilon}\, \widehat{b}_0 \, e^{-i\widehat{H}t/\varepsilon}$. Let $a_0 := \pi_{\mathrm{r}} \, u_0^* \, b_0 \, u_0 \, \pi_{\mathrm{r}}$ and define $a_0(t)$ is in (61). Then for each $T < \infty$ there is a constant $C_T < \infty$ such that for all $t \in [-T, T]$*

$$\|(B(t) \; - \; \mathcal{W}_\varepsilon(u_0 \, a_0(t) \, u_0^*))\Pi\| \; \leq \; \varepsilon \, C_T \, . \tag{71}$$

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 (71) that

$$\Big\|(B(t) \; - \; \widehat{b_0(\Phi^t)})\Pi\Big\| \; \leq \; \varepsilon \, C_T \, .$$

Corollary 6.2 follows from Theorem 6.1 and a straightforward expansion in ε of the terms to be estimated after rotation with U.

7 The Dirac equation

7.1 Adiabatic decoupling of electrons and positrons

We apply the adiabatic perturbation theory to the one-particle Dirac equation with slowly varying external potentials, i.e. to

$$\widetilde{H}_{\mathrm{D}} = c\alpha \cdot \Big(-i\hbar\nabla_y - \frac{e}{c} A(\varepsilon y)\Big) + \beta mc^2 + e\phi(\varepsilon y)$$

acting 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 $B = \nabla \wedge A$ and $\phi : \mathbb{R}^3 \to \mathbb{R}$ the potential of an external electric field $E = -\nabla\phi$. For the Dirac matrices α, β we make the standard choice

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

where $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ denotes the vector of the Pauli spin matrices. The small parameter $\varepsilon > 0$ controls the variation of the external potentials. To keep track of the size of the error terms, in this section all physical constants, including $\hbar$, are displayed.

Transforming to the macroscopic space-scale $x = \varepsilon y$ one obtains the Dirac Hamiltonian

$$\widehat{H}_{\mathrm{D}} = c\alpha \cdot \Big(-i\varepsilon\hbar\nabla_x - \frac{e}{c} A(x)\Big) + \beta mc^2 + e\phi(x) \tag{72}$$

and we are interested in the solution of the time-dependent Dirac equation for times of order ε^{-1}, i.e. in solutions of

$$i\,\varepsilon\hbar \frac{\partial}{\partial t} \psi_t = \widehat{H}_{\mathrm{D}} \, \psi_t \tag{73}$$

for $|t| = \mathcal{O}(1)$. The solutions of (73) for small ε approximately describe the dynamics of electrons, resp. positrons, in weak fields, as in storage rings, accelerators, or cloud chambers, for example.

$\widehat{H}_{\mathrm{D}}$ is the Weyl quantization of the matrix-valued function

$$H_{\mathrm{D}}(q,p) = c\alpha \cdot \left(p - \frac{e}{c}A(q)\right) + \beta mc^2 + e\phi(q)$$

on phase space $\mathbb{R}^6$, where now Weyl quantization is in the sense of $p \mapsto -i\varepsilon\hbar\nabla_x$, i.e. on the right hand side of (5) ε must be replaced by $\varepsilon\hbar$. $\hbar$ appears here for dimensional reasons and is a fixed physical constant. The small parameter of the space-adiabatic expansion is ε. $H_{\mathrm{D}}(q,p)$ has two two-fold degenerate eigenvalues

$$E_{\pm}(q,p) = \pm c p_0(q,p) + e\phi(q)$$

with the corresponding eigenprojections

$$P_{\pm}(q,p) = \frac{1}{2}\left(1 \pm \frac{1}{p_0(q,p)}\left(\alpha\cdot\left(p - \frac{e}{c}A(q)\right) + \beta mc\right)\right),$$

where $p_0(q,p) = \sqrt{m^2c^2 + (p - \frac{e}{c}A(q))^2}$. Obviously

$$E_{+}(q,p) - E_{-}(q,p) = 2cp_0(q,p) \geq C\langle p\rangle > 0\,,$$

whenever A is uniformly bounded. Therefore the corresponding subspaces are adiabatically decoupled and the effective dynamics on each of them can be computed using our general scheme. 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 the assumptions from Section 3 are satisfied. In particular, $\widehat{H}_{\mathrm{D}}$ is essentially self-adjoint on $\mathcal{S}(\mathbb{R}^4, \mathbb{C}^4)$ and $\widehat{E}_{\pm}$ on $\mathcal{S}(\mathbb{R}^4)$.

To be consistent with the notation from the previous sections, let $\pi_0(q,p) = P_+(q,p)$ 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 $\mathrm{Ran}\pi_0(q,p)$. Since the degeneracy of $\mathrm{Ran}\pi_0(q,p)$ is related to the spin of the electron, a natural choice is the σ_z-representation with respect to the "mean"-spin $S(q,p)$ which commutes with $H_{\mathrm{D}}(q,p)$ [FoWo, Th]. The eigenvectors $\psi_\pm(q,p)$ of the operator $e_3\cdot S(q,p)$ in $\mathrm{Ran}\pi_0(q,p)$ are

$$\psi_+(q,p) = c\sqrt{\frac{p_0}{2(p_0+mc)}}\begin{pmatrix} p_0^{-1}(p_0+mc) \\ 0 \\ v_3 \\ v_1+iv_2 \end{pmatrix}, \quad \psi_-(q,p) = c\sqrt{\frac{p_0}{2(p_0+mc)}}\begin{pmatrix} 0 \\ p_0^{-1}(p_0+mc) \\ v_1-iv_2 \\ -v_3 \end{pmatrix}.$$

We abbreviated $v(q,p) := c\,(p - \frac{e}{c}A(q))/p_0(q,p)$ for the velocity. The relevant part of u_0 for the analysis of the electron band is thus given by $u_0(q,p) = (\psi_+(q,p), \psi_-(q,p), *, *)$

with $u_0 \in S^0_1$. 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 $\widehat{h}_{\rm e} := \Pi_{\rm r}\,\widehat{h}\,\Pi_{\rm r}$ up to arbitrary order.

An alternative way to arrive at the same $u_0(q,p)$ is to note that the Foldy-Wouthuysen transformation $u_{\rm FW}(p)$, c.f. [FoWo], diagonalizes the free Dirac Hamiltonian $H_0(p)$, i.e. $H_{\rm D}$ with $A, \phi \equiv 0$. Including the fields $u_0(q,p) = u_{\rm FW}(p - \frac{e}{c}A(q))$ then diagonalizes $H_{\rm D}(q,p)$.

For the principal symbol of $h_{\rm e}$ one finds of course

$$h_{{\rm e},0}(q,p) = E_+(q,p)\mathbf{1}_{\mathbb{C}^2}\,.$$

For the subprincipal symbol after a lengthy but straightforward calculation our basic formula (45) yields

$$h_{{\rm e},1}(q,p) = -\frac{\hbar e}{2p_0(q,p)}\,\sigma\cdot\left(B(q) - \frac{p_0}{c\,(p_0(q,p)+mc)}\,v(q,p)\wedge E(q)\right) =: -\frac{\hbar}{2}\,\sigma\cdot\Omega(q,p)\,. \tag{74}$$

Note that the factor $\hbar$ comes from the fact that the nth term in the space-adiabatic expansion carries a prefactor $\hbar^n$. Defining

$$\gamma(q,p) = 1/\sqrt{1-(v(q,p)/c)^2} = p_0(q,p)/(mc)$$

one concludes that

$$\Omega(q,p) = \frac{e}{mc}\left(\frac{1}{\gamma(q,p)}\,B(q) - \frac{1}{c\,(1+\gamma(q,p))}\,v(q,p)\wedge E(q)\right)\,. \tag{75}$$

We remark that the second term in (45), the "Berry term", does not coincide with the second term in (75), in contrast to the claim in [BoKe$_1$]. Indeed, the compact expression (75) is obtained only through cancellations in more complicated expressions coming from both terms contributing in (45).

We summarize our results on the adiabatic decoupling and the effective dynamics for the Dirac equation in the following

Theorem 7.1 *Let $A \in C^\infty_{\rm b}(\mathbb{R}^3,\mathbb{R}^3)$ and $\phi \in C^\infty_{\rm b}(\mathbb{R}^3,\mathbb{R})$. Then there exist orthogonal projectors $\Pi_\pm$ with $\Pi_+ + \Pi_- = \mathbf{1}$ such that $[\widehat{H}_{\rm D},\Pi_\pm] = \mathcal{O}_0(\varepsilon^\infty)$, and there exists a unitary U and $\widehat{h} \in {\rm OP}S^1_1$ with*

$$\widehat{h} = \begin{pmatrix} \widehat{h}_{\rm e} & 0 \\ 0 & \widehat{h}_{\rm p}\end{pmatrix}\,, \tag{76}$$

such that

$$e^{-i\widehat{H}_{\rm D}t} - U\,e^{-i\widehat{h}t}\,U^* = \mathcal{O}_0(\varepsilon^\infty|t|)\,. \tag{77}$$

Here $\widehat{h}_{\rm e}$ and $\widehat{h}_{\rm p}$ are semiclassical operators on $L^2(\mathbb{R}^3,\mathbb{C}^2)$ with $h_{\rm e}(q,p,\varepsilon) \asymp E_+(q,p)\mathbf{1}_{\mathbb{C}^2} + \sum_{j=1}^\infty \varepsilon^j\,h_{{\rm e},j}(q,p)$ and $h_{{\rm e},j} = \pi_{\rm r}(u^*\,\#\,H_{\rm D}\,\#\,u)_j\pi_{\rm r} \in S^{1-j}_1(\mathcal{B}(\mathbb{C}^2))$ for all $j \geq 0$, where $u \in S^0_1(\varepsilon)$ is constructed as in Section 4. In particular, $h_{{\rm e},1}(q,p)$ is given by (74) and thus

$$\widehat{h}_{\rm e} = \left(c\sqrt{m^2c^2 + (-i\varepsilon\hbar\nabla - \frac{e}{c}A(x))^2} + e\phi(q)\right)\mathbf{1}_{\mathbb{C}^2} \,-\, \varepsilon\,\frac{\hbar}{2}\,\sigma\cdot\widehat{\Omega(q,p)} \,+\, \mathcal{O}_0(\varepsilon^2)\,. \tag{78}$$

Analogous results hold for $h_{\rm p}$. The errors in (77) and (78) 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 (78) 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$_2$] 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$_2$], nonsystematic expansions are [DeKo] and [HeBa].

We close this section with an important issue, which so far has been ignored completely. To decide whether the space-adiabatic approximation is appropriate in a concrete problem one needs a, at least heuristic, formula for the dimensionless constant ε. Let us consider an arbitrary band function $E_{\mathrm{r}}(q,p)$ with $\Delta E(q,p) > 0$ the size of the gap. Then $t_{\mathrm{m}} = \hbar/\Delta E(q,p)$ defines, locally in phase space, the microscopic time scale. Since for any eigenfunction of $H_0(q,p)$ with eigenvalue $E_{\mathrm{r}}(q,p)$

$$\nabla\psi(q,p) = -\left(H_0(q,p) - E_{\mathrm{r}}(q,p)\right)^{-1}\nabla\left(H_0(q,p) - E_{\mathrm{r}}(q,p)\right)\psi(q,p)\,,$$

one obtains from (45) with $H_1 = 0$ that

$$\|\,\pi_{\mathrm{r}}\,h_1(q,p)\,\pi_{\mathrm{r}}\,\| \approx \frac{\hbar\,|\nabla_p E_{\mathrm{r}}(q,p)|\,|\nabla_q E_{\mathrm{r}}(q,p)|}{\Delta E(q,p)}\,.$$

The norm of h_1 measured in units given by the size of the gap is an indicator for the numerical value of ε and hence

$$\varepsilon(q,p) := \frac{\|\,\pi_{\mathrm{r}}\,h_1(q,p)\,\pi_{\mathrm{r}}\,\|}{\Delta E(q,p)} \approx \frac{\hbar\,|\nabla_p E_{\mathrm{r}}(q,p)|\,|\nabla_q E_{\mathrm{r}}(q,p)|}{\left(\Delta E(q,p)\right)^2}\,. \tag{79}$$

At first glance it might be surprising to have ε to depend on the region in phase space. But in fact such a dependence is very natural. For example, in the Born-Oppenheimer setting the adiabatic decoupling becomes poor for large momenta.

For the Dirac equation (79) yields

$$\varepsilon_{\mathrm{D}} \le \frac{\hbar e}{4c^3 m^2}\left(|\nabla A| + |\nabla\phi|\right) \approx 10^{-9}\,B[\mathrm{T}] + 10^{-17}E[\mathrm{V/m}]\,.$$

The electric field strength E in the laboratory devices hardly exceeds 10^7V/m, which would correspond to $\varepsilon_E \le 10^{-10}$, and the magnetic field strength B reaches at most 10T yielding $\varepsilon_B \le 10^{-8}$. Thus, since $t_{\mathrm{m}} \approx 10^{-19}s$, the second order term $h_{\mathrm{e},2}$ of the space-adiabatic expansion is expected to become important for times on the order of seconds, compare with (35) and (37). The space-adiabatic approximation of the Dirac equation has a rather wide range of validity. It only breaks down in fields near nuclei or charged elementary particles.

7.2 The semiclassical limit of the Dirac equation

Equipped with $h_{\mathrm{e},0}$ and $h_{\mathrm{e},1}$ we can apply the general results of Section 6 on the semiclassical limit to the Dirac equation. Let $\Phi^t_\pm$ be the Hamiltonian flows generated by $E_\pm(q,p)$

on phase space $\mathbb{R}^6$ and let $\widehat{B} = \widehat{b}\,\mathbf{1}$, $b \in S^0_1(\mathbb{R})$, be a semiclassical observable in the unrotated Hilbert space which does not depend on spin. From Corollary 6.2 we conclude for each $T < \infty$ the existence of a constant C_T such that for all $t \in [-T, T]$

$$\Big\| \Big(B(t) - \mathcal{W}_\varepsilon(b(\Phi^t_+))\,\mathbf{1} \Big) \Pi_+ \Big\| \leq \varepsilon\, C_T \quad \text{and} \quad \Big\| \Big(B(t) - \mathcal{W}_\varepsilon(b(\Phi^t_-))\,\mathbf{1} \Big) \Pi_- \Big\| \leq \varepsilon\, C_T\,,$$

where $B(t) = e^{i\widehat{H}_{\mathrm{D}}t/(\varepsilon\hbar)}\,\widehat{B}\,e^{-i\widehat{H}_{\mathrm{D}}t/(\varepsilon\hbar)}$. Hence, to leading order, states in the range of Π_+ behave like classical relativistic electrons and states in the range of Π_- like classical relativistic positrons. We emphasize that, in general, $\Pi_\pm$ 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 (78) a natural choice is to take as spin operator the vector of Pauli-matrices σ in the rotated electronic subspace. In the original Hilbert space this amounts to

$$\Sigma = U \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix} U^* = \frac{2}{\hbar}\,\widehat{S} + \mathcal{O}(\varepsilon)\,,$$

where $S(q,p)$ is the "mean" spin defined before.

The leading order semiclassical approximation for $\sigma(t) = e^{i\widehat{h}_{\mathrm{e}}t/(\varepsilon\hbar)}\,\sigma\,e^{-i\widehat{h}_{\mathrm{e}}t/(\varepsilon\hbar)}$ follows from Theorem 6.1. For each $T < \infty$ there is a constant $C_T < \infty$ such that for $t \in [-T, T]$

$$\|\sigma(t) - \widehat{\sigma_0(t)}\| \leq \varepsilon\, C_T\,, \tag{80}$$

where $\sigma_{0k}(q,p,t)$, $k \in \{1,2,3\}$, is obtained as the solution of

$$\frac{\partial\, \sigma_{0k}(q,p,t)}{\partial t} = -\,\frac{i}{2}\Big[\, \sigma \cdot \Omega(\Phi^t_+(q,p)),\ \sigma_{0k}(q,p,t)\,\Big] \tag{81}$$

with initial condition $\sigma_{0k}(q,p,0) = \sigma_k$. This follows from the Equations (61) and (62) by setting $\sigma_{0k}(q,p,t) = D^*(q,p,t)\,\sigma_k\,D(q,p,t)$.

To solve Equation (81) one makes an ansatz $\sigma_{0k}(q,p,t) = s_k(q,p,t)\cdot\sigma$ with $s_k(q,p,0) = e_k$. Using $[\sigma_n, \sigma_m] = 2\,i\,\varepsilon_{nmk}\,\sigma_k$, one finds that the spin- or "magnetization"-vector $s_k(q,p,t)$ is given as the solution of

$$\frac{\partial\, s_k(q,p,t)}{\partial t} = -\,s_k(q,p,t)\,\wedge\,\Omega(\Phi^t_+(q,p))\,. \tag{82}$$

(82) is the BMT-equation [BMT, Ja] on the level of observables. It was derived by Bargmann, Michel and Telegdi in 1959 on purely classical grounds as the simplest Lorentz invariant equation for the spin dynamics of a classical relativistic particle.

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 6, 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. A non-rigorous 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 $U^*\,\widehat{H}_{\mathrm{D}}U$ are isospectral and since (77) 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 6, the latter is somewhat easier to obtain. In [GMMP, Sp] the semiclassical limit of the Dirac equation is discussed using matrix-valued Wigner functions. Their results hold for an arbitrary macroscopic time interval, but fuse, as does the WKB approach, adiabatic and semiclassical limit. No higher order corrections seem to be accessible and the results are weaker than ours in the sense that the approximations do not hold uniformly in the states.

This leads us to the next natural question: What can be said about higher order corrections? While in general one would need $h_{\mathrm{e},2}$, according to (59) the semiclassical limit of observables of the type $\widehat{b} = \widehat{b}_0 \mathbf{1}_{\mathbb{C}^2}$, $b_0 \in S^0_1(\mathbb{R})$, can be determined without this explicit information. For such a scalar symbol the principal symbol $b_0(t)$, i.e. the solution to (58), will remain scalar and thus its commutator with $h_{\mathrm{e},2}$ in (59) vanishes identically for all times. The solution $b_1(t)$ of (59) 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 $x_0(q,p,t) = x_0(\Phi^t_+(q,p))$ and $x_1(t)$ is obtained, according to Equation (59), as the solution of

$$\frac{d\,x_1(t)}{dt} = \{E_+\mathbf{1}, x_1(t)\} + i[h_{\mathrm{e},1}, x_1(t)] - \{h_{\mathrm{e},1}, x_0(t)\} \tag{83}$$

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

$$\{h_{\mathrm{e},1}, x_0(t)\} = -\frac{\hbar}{2}\,\sigma \cdot \{\,\Omega, x_0(t)\}\,, \tag{84}$$

which is not scalar and thus responsible for the splitting of trajectories of electrons with distinct spin orientation. Hence, as in (65),

$$x_1(t) = -\frac{\hbar}{2}\int_0^t ds\,\mathcal{U}(t-s)\,\sigma \cdot \{\,\Omega,\, x_0(s)\}\,,$$

where $\mathcal{U}(t)$ is the "classical flow" defined through (63).

Without claim of rigor, we observe in (75) 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

$$\frac{\hbar}{2}\,\sigma \cdot \{\Omega, x_0(t)\} = \frac{\hbar e}{2mc}\sigma_z \frac{\partial B}{\partial q_z}\frac{\partial \Phi^t_q}{\partial p_z} = t\,\frac{\hbar e}{2m^2 c}\begin{pmatrix} b & 0 \\ 0 & -b \end{pmatrix}$$

and thus according to (83), (84) 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.

8 Conclusions

The basic formulae (41), (42) can be applied, in essence in a mechanical fashion, to any concrete quantum problem with two provisos. First of all the problem has to be cast into the general form (1) and secondly one must have sufficient information on the principal symbol $H_0(q,p)$. Depending on H_0 considerable simplifications of (41), (42) may be in force, one example being the effective Hamiltonian of the time-adiabatic theorem studied in Section 5.4. As a net result, if the conditions of the space-adiabatic Theorem 3.1 are satisfied, the full Schrödinger equation is approximated by an effective Schrödinger equation referring to a specific relevant energy band. The errors are estimated and, in general, the time scale of validity is much larger than the one which can be reached within a semiclassical approximation.

We focused our interest on a single relevant energy band. No information on the complement is needed except for global quantities like the resolvent $(H_0(q,p)-E_{\mathrm{r}}(q,p))^{-1}(1-\pi_0(q,p))$. In previous investigations [Bl_1, LiFl] all energy bands are treated simultaneously. An example which would not fall under such a scheme is nonrelativistic QED, which governs electrons coupled to the quantized radiation field. In this case the principal symbol has a two-fold degenerate eigenvalue at the bottom of the spectrum separated by a gap from the continuous spectrum, provided $|p|$ is sufficiently small and there is a suitable infrared cutoff [PST_1].

The main restriction of our work is the gap condition of Section 3. There are two standard mechanisms of how this condition is violated. (1) There are two (or possibly more) locally isolated energy bands of constant multiplicity which cross on a lower dimensional submanifold. Away from the crossing region the wave function in one band is governed by the effective Hamiltonian discussed before. If the wave function comes close to the crossing manifold, there is a certain probability to make a transition to the other band. In rather specific model systems such transitions have been studied in considerable detail [Ha_2, HaJo_1, FeGe, FeLa]. (2) H_0 has a smooth band of constant multiplicity bordering the continuous spectrum *without* gap. This is the rule in models from nonrelativistic QED with massless photons. Results for the massless Nelson model [Te_1] indicate that smoothness of $\pi_0(q,p)$ suffices also in general for adiabatic decoupling at leading order with intraband dynamics generated by $h_0+\varepsilon h_1$ as defined by (44). However, the expansion stops at this stage. Physically, the electron looses energy through radiation, which means that the next order correction must be dissipative.

From the physics point of view the dynamics of molecules and the dynamics of electrons in a solid are the two most prominent areas of application for the space-adiabatic perturbation theory. The former has been discussed already in Section 5.3. Bloch electrons do not quite fall into our scheme, since the classical phase space is $\mathbb{R}^d \times \mathbb{T}^d$, $\mathbb{T}^d$ a flat d-dimensional torus. This will require some changes which are discussed in [PST_2].

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