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Space-adiabatic decoupling in Quantum Dynamics

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Preface

In many physical situations, separation of scales plays a fundamental role in understanding the dynamical behavior of the system. In particular, we focus on physical systems in which it is possible to distinguish between fast and slow degrees of freedom. The goal is to obtain an effective Schrödinger equation governing the dynamics of the slow degrees of freedom, thereby greatly simplifying the complexity of the problem.

The previous lines summarize the spirit and the goals of the theory outlined in this thesis. The thesis collects original results obtained as a joint work with Herbert Spohn and Stefan Teufel, who initiated this research project some years before and introduced me into this field of research. The results have been obtained during the second part of my Ph. D. studies at SISSA, Trieste, under the internal supervision of Gianfausto Dell'Antonio.

Since the reader will be probably looking forward to read the main body of the thesis, I will spend just few more words about the novelty of the results and the references to the literature.

As far as the novelty of the results is concerned, all the results appearing in the main body of the thesis are essentially new, with the exception of Egorov's theorem in Ch.2 and few minor propositions. As opposed, the results reviewed in the Appendix appeared already in the literature, see for example [Hö, Fo, Iv, GMS].

Detailed references to the literature and to related approaches will be given sectionwise, so that the comparison of the methods and the results will be easier. However, I wish to mention here that the results in [EmWe, NeSo] have been greatly inspiring for us.

At the risk of being pedantic, I wish to emphasize that *all the results should be considered as the fruit of a joint work with Herbert Spohn and Stefan Teufel*, although this will not be explicitly mentioned sectionwise.

The introductory chapter looks very much as the transcription of the talk I had the occasion to give in many places (Vienna, Taxco, Trieste, Rome, Cala Gonone, Bielefeld,...) in the last months. Indeed it is. But this is a consequence of the precise choice to make the first chapter as readable as possible, so that I

avoided any use of technical concepts in the Introduction. This is also the reason why references to the literature do not appear in the introduction.

Finally, I took for myself the freedom to break a very solid convenction. Indeed, in this thesis the word "hamiltonian" is written without the capital letter, since in the last eight years - since my first course in rational mechanics - nobody was able to explain to me why the words "algebraic", "bosonic", "euclidean" or "fermionic" are usually written in small letters, while "hamiltonian" should be promoted to the capital letter. I hope that Sir Hamilton will not be too much offended for that and, more important, will not take this fact too seriously.

Miramare, Trieste,
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Gianluca Panati

Acknowledgements

The last day before the conclusion of a thesis is probably the right occasion to look back and to think about all the people who helped me during these years.

My thought goes, first of all, to my father, who taught me the love for knowledge and research, and the fact that "books are written by human beings". To his dear memory, I wish to dedicate this thesis.

I am very much indebted to my teachers. Looking back many years ago, I wish to thank Prof.sa Castagnetti, from whom I learned the love for clearness of reasoning. As for the years at university, I wish to remember Prof. Paganoni, Prof. Rigoli, Prof. Valz Gries, Prof. Lanz and Prof. Cantoni who greatly contributed to introducing me in the mysteries of mathematics and physics. But I wish specially to thank Luigi Galgani, whose enthusiasm and passion for mathematical physics have deeply fascinated many students, including me.

As for the recent past, I am very indebted to Gianfausto Dell'Antonio, who introduced me to the world of scientific research and, as a middle-age painter, has been teaching me day-by-day the art of doing research. I am also grateful to the people in his "delocalized group", namely Rodolfo Figari, Sandro Teta, Riccardo Adami and Domenico Finco, for their friendship and for many interesting discussions.

I am very grateful to Herbert Spohn, who taught me the importance of combining the mathematical rigor with a deep insight into the physical problems and who introduced me to the realm of adiabatic problems in quantum physics. I also appreciated very much his constant encouragement in the last two years.

Last but not least, I wish to thank Stefan Teufel for his friendship and for the day-by-day "friendly competition" who greatly accelerated the progress of this work. And for listening to me, when I tried to convince him that reality does not exist...

Finally, I wish to thank my relatives and all my friends, both in Trieste and in München, for the "healthy distractions" during the preparation of this thesis. Without them, I would have gone crazy many months ago....

A special thanks to Sarah Joy for providing me the music, her music, that I mostly listened to during the typing of this thesis.

Contents

Chapter 1

Introduction

In the dynamics of many classical and quantum systems a multi-scale dynamics appears, i.e. there is a clear distinction between "fast" and "slow" degrees of freedom. As a consequence of the separation of time-scales, or equivalently of energy scales, the fast degrees of freedom readjust almost instantaneously and without an appreciable exchange of energy to the dynamics of the slow ones. This physical situation, well known both in classical and quantum physics, is summarized under the name of **adiabatic decoupling**, where the greek root $\acute{\alpha}$ (=not)-$\delta\iota\acute{\alpha}$ (=through)-$\beta\alpha\acute{\iota}\nu\omega$ (=to pass, to penetrate) reminds us that exchanges are negligible on the microscopic time scale. Clearly, the previous claims can be made precise by introducing a suitable dimensionless parameter $\varepsilon \ll 1$ which roughly correspond, by the physical viewpoint, to the ratio between the typical time scale for fast and slow degrees of freedom.

The phenomenon of adiabatic decoupling appears in a great variety of physical systems. Focusing on the realm of quantum systems, we consider the following ones.

Ex.1 Molecular physics The first and prototypical example of adiabatic decoupling in a quantum system comes from molecular physics. Indeed, in the spirit of the well-known Born-Oppenheimer approximation, one expects that in a molecule the fast electron dynamics adiabatically readjusts to the slow motion of the nuclei.

Ex.2 Electron dynamics The second relevant example of adiabatic decoupling appears if we consider an electron, moving in a *slowly varying* external electromagnetic potential, as, for example, in a storage ring or in a cloud chamber. Roughly speaking, the term *slow variation* means that the scale of the space variation of the potentials is much larger that the Compton wavelenght of the electron at the typical energy scale (see Sec.?? for a detailed discussion). In this physical situation one expects that the dynamics

of the translational degrees of freedom (position and momentum) is much slower than the dynamics of other internal degrees of freedom. What are the internal degrees of freedom? The answer depends on the particular model one is considering.

Ex. 2.1 Pauli electron If the electron dynamics is described by the (relativistic) Pauli equation then the internal fast degrees of freedom are simply given by the two-component Pauli spin. One expects that, for slowly varying external potentials, the Pauli spin has a fast precession around the direction of the instantaneous magnetic field, which varies slowly in time because of the slow translational motion. Although a separation of time-scales appears, this example is not really interesting for us, since the fast and slow degrees of freedom are already decoupled at the leading order.

Ex. 2.2 Dirac electron For a particle described by the Dirac equation the internal degrees of freedom corresponding to four-component Dirac spin can be regarded, from the physical viewpoint, as a combination of a *discrete* degree of freedom corresponding to the electron-positron duality and the degrees of freedom associated with the physical Pauli spin. This example will be discussed in full detail in Ch. 3.

Ex. 2.3 Pauli-Fierz electron A more sophisticated model should take into account the interaction of the electron with the self-generated (quantized) electromagnetic field. A mathematically rigorous model describing this situation is the Pauli-Fierz model (see Sec. 4.1) sometimes called *non-relativistic QED*. In this case both the dynamics of the photon cloud dynamics and the spin dynamics adiabatically readjust to the slow translational motion. This example is outlined in detail in Ch. 4.

Ex.3 Constrained motion It is an old problem in mathematical physics to determine effective equations of motion for a particle which is constrained to a smooth submanifold Σ of the configuration space through strong external confining forces. Following a remark in [Te], we notice that this problem is related to a separation of time-scales. Indeed, one expects that, for strong confining forces, the dynamics in the direction transverse to Σ is much faster than the longitudinal dynamics, the ratio of the time-scales being related to the steepness of the confining potential. [1]

[1] To avoid confusion, a remark is due. Usually, see [FrHe], the limit of strong confinement is realized through dilations in the transverse direction. At the level of classical mechanics one can equivalently rescale the tangential direction by the opposite factor obtaining, up to a total rescaling of space-time, the same limit dynamics. However at the quantum mechanical level

Ex.4 Bloch electron A subtler example, in which the separation of time scales is not clear a priori, appears when one considers an electron in a periodic crystal with an external *slowly varying* electromagnetic potential. Here it is assumed that the scale of variation of the external potential is much larger than the lattice scale. It is part of the common lore in solid state physics, that in this physical situation the dynamics of the wavefuction at the macroscale is much slower than the dynamics at the lattice scale, and that the latter adiabatically readjust to the first one. The first rigorous proof of this fact and of the related Peierl's substitution has been obtained in and is given in Ch. 6

The ultimate goal of our theory is to prove that, in all the previous examples, the dynamics of the slow degrees of freedom is decoupled from the dynamics of the fast ones **(adiabatic decoupling)** and to give an algorithm to compute an effective hamiltonian governing the motion of the slow ones to an arbitrary order of approximation **(adiabatic perturbation theory)**. Moreover, in this thesis we outline a model-independent technique, developed in [PST$_1$], which is in our opinion vastly superior to a case by case study.

The first step of our analysis is the observation that all the previous examples share the same mathematical structure, which can be nicely expressed by using the operator-valued Weyl quantization (summarized in Appendix A) or a suitable newly developed extension of it (see Ch. 5) in the case of the Bloch electron. The common mathematical structure can be summarized in the following terms:

(i) the Hilbert space $\mathcal{H}$ corresponding to the pure states of the quantum system can be decomposed, after a suitable unitary transformation, as the tensor product

$$\mathcal{H} \cong L^2(X) \otimes \mathcal{H}_{\rm f} \tag{1.1}$$

where X denotes the classical configuration space for the slow degrees of freedom and $\mathcal{H}_{\rm f}$ is a (separable) Hilbert space corresponding to the fast degrees of freedom. Notice that in Ex.1 and 2.x one has simply $X = \mathbb{R}^d$ for a suitable d.

(ii) from the parameters appearing in the hamiltonian operator H^ε describing the full dynamics of the system can be extracted a dimensionless parameter $\varepsilon \ll 1$ *and*

(iii) the operator H^ε is the ε-Weyl quantization of an operator valued symbol $H(q,p)$ defined on the classical phase space T^*X for the slow degrees of freedom. (This is not literally true in Ex.4 where one should consider,

the two approaches are not equivalent anymore. The second approach, which in a sense better describe the physical situation, fits in the framework of space-adiabatic theory.

more generally, morphism of an Hilbert-space bundle over the phase space $T^*X \cong \mathbb{T}^d \times \mathbb{R}^d$)

It is convenient to work out in full detail two simple examples.

Ex.1 Molecular physics. Let us consider a molecule with n nuclei and n_e electrons. The Hilbert space for the corresponding quantum theory (neglecting spin considerations) is given by $\mathcal{H} = L^2(\mathbb{R}^{3n}) \otimes L^2(\mathbb{R}^{3n_e})$, so that the splitting (1.1) is trivial, with $\mathcal{H}_{\rm f}$ simply given by the electronic Hilbert space. Let denote with $x = (x_1, \ldots, x_n) \in \mathbb{R}^{3n}$ the nuclei configuration and with $y = (y_1, \ldots, y_{n_e}) \in \mathbb{R}^{3n_e}$ the electrons configuration. Assuming for simplicity that all the nuclei have the same mass M, the full hamiltonian is given by

$$H_{\rm mol} = -\frac{\hbar^2}{2M}\Delta_x - \frac{\hbar^2}{2m_e}\Delta_y + V_n(x) + V_{ne}(x,y) + V_e(y) \tag{1.2}$$

where V_n contains the nuclei repulsion, V_e the electrons repulsion and $V_{ne}(x,y)$ the electron-nuclei interaction. Here the interaction can be the Coulomb potential or any other convenient interaction (e.g. Coulomb interaction smeared out with the nuclear form factor). By introducing natural units ($m_e = 1 = \hbar$) and the adiabatic parameter $\varepsilon = \sqrt{m_e/M} \ll 1$, the hamiltonian can be rewritten as

$$H^\varepsilon_{\rm mol} = -\frac{\varepsilon^2}{2}\Delta_x + H_{\rm el}(x) \tag{1.3}$$

where $H_{\rm el}(x)$ is the electronic hamiltonian for a given configuration of the nuclei,

$$H_{\rm el}(x) = -\frac{1}{2}\Delta_y + V_n(x) + V_{ne}(x,y) + V_e(y) \tag{1.4}$$

From (1.3) it is evident that $H^\varepsilon_{\rm mol}$ is the ε-Weyl quantization of the symbol

$$H_{\rm mol}(q,p) = p^2 1_{\mathcal{H}_{\rm f}} + H_{\rm el}(q), \tag{1.5}$$

which takes values in the space of the (eventually unbounded) operators over $\mathcal{H}_{\rm f}$. Notice that, apart from the fact that one has to face the unboundness of the operators, this example is, from a certain viewpoint, very simple. Indeed, in (1.5) the non-scalar part of the symbol, depends only on one of the canonical variables. This yields a major simplification, as will be pointed out in Sec. 2.4.3.

Ex.2 Dirac equation. The first interesting example in which the non-scalar part of the symbol depends on both the canonical variables appears when one considers the Dirac equation. The Hilbert space of the quantum theory

is simply given by $L^2(\mathbb{R}^3, \mathbb{C}^4)$ so that the splitting (1.1) is again trivial, with $\mathcal{H}_{\rm f} = \mathbb{C}^4$ and $X = \mathbb{R}^3$. In a fixed reference frame, the Dirac dynamics is given by

$$i\hbar\partial_t\psi_t = \tilde{H}_{\rm D}\psi_t \tag{1.6}$$

with

$$\tilde{H}_{\rm D} = c\alpha\cdot\left(-i\hbar\nabla_y - \frac{e}{c}A(\varepsilon y)\right) + \beta mc^2 + eV(\varepsilon y)$$

Here α and β are the Dirac matrices in Pauli representation, i.e.

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

where $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ denotes the vector of the Pauli spin matrices. The functions $A \in C^\infty_{\rm b}(\mathbb{R}^3, \mathbb{R}^3)$ and $V \in C^\infty_{\rm b}(\mathbb{R}^3, \mathbb{R})$ are the potentials of an external electromagnetic field and the dimensionless parameter $\varepsilon \ll 1$ express mathematically the physical assumption that the potentials are slowly varying on the microscopic space scale. It is convenient to switch to macroscopic units $x = \varepsilon y$ and $s = \varepsilon t$ so that the hamiltonian can be rewritten (in natural units $\hbar = 1 = c$) as

$$\widehat{H}_{\rm D} = \alpha\cdot(-i\varepsilon\nabla_x - eA(x)) + m\beta + eV(x) \tag{1.7}$$

and one has to consider the Schrödinger equation

$$i\,\varepsilon\partial_s\psi_s = \widehat{H}_{\rm D}\,\psi_s \tag{1.8}$$

for macroscopic times of order 1, i.e. $|s| = \mathcal{O}(1)$. It is clear that $\widehat{H}_{\rm D}$ is the ε-Weyl quantization of the matrix-valued function

$$H_{\rm D}(q,p) = \alpha\cdot(p - eA(q)) + m\beta + eV(q)$$

defined on the phase space $T^*X \cong \mathbb{R}^6$.

In other examples the Hilbert space splitting (1.1) can be not evident *a priori*. For example, in the case of the Pauli-Fierz electron (Ex. 2.3, see Ch.4) the splitting becomes apparent only after a unitary transformation to the representation for which the total momentum (electron + photon field) is diagonal. For the Bloch electron (Ex. 4, see Ch 6) a convenient form of the Bloch-Floquet transformation is required.

By considering the spectrum of the operator $H(q,p)$, regarded as an (eventually unbounded) operator over $\mathcal{H}_{\rm f}$, when (q,p) varies over the classical phase space the typical **band structure** appears. Moreover, in many cases, there is a phisically relevant band which is uniformly separated from the remainder of the

spectrum (see Sec. 2.1 for a precise condition). This will be called the **relevant band**.

It is worthwhile to mention that the mathematical structure summarized in (i)-(iii) can be regarded as the starting point for the usual quantum adiabatic theory, that in the context of the present thesis will be referred to as the **time-adiabatic theory**. Indeed, in the spirit that the slow degrees of freedom are *classical* degrees of freedom, one considers a given path (q_t, p_t) in the classical phase space T^*X, as for example the flow induced by a classical hamiltonian. Then one considers the Schrödinger equation in $\mathcal{H}_{\rm f}$

$$i\partial_t\varphi_t = H(q_t, p_t)\varphi_t =: \tilde{H}(\varepsilon t)\varphi_t, \qquad \varphi_0 \in \mathcal{H}_{\rm f}, \tag{1.9}$$

where the parameter ε appears as a consequence of the slow variation of (q_t, p_t). But equation (1.9) is nothing but a Schrödinger equation in $\mathcal{H}_{\rm f}$ with a *slowly time-dependent* hamiltonian $\tilde{H}$, i.e. the starting point of the usual time-adiabatic theory[2](see references).

In this thesis we assume a different point of view: *all* the degrees of freedom are considered quantum mechanical and the adiabatic decoupling is carefully distinguished from the semiclassical limit. This approach has been baptized **space-adiabatic approach** in [SpTe]. The use of the word *space* fits many different interpretations: for example, it is related to the fact that in many situation (Ex. 2.x-3-4) the external potentials have a a slow variation in space which induces the separation of time-scales; alternatively, it can be related to the fact that, by using microlocal analysis, we develop an adiabatic theory over the classical phase space ($\simeq$ space) rather than over the time axis ($\simeq$ time).

The goals, and the results[3], of the space adiabatic theory can be summarized in the following scheme:

A. Existence of almost invariant subspace. The first goal in space-adiabatic theory is to show that **interband transitions** are exponentially small in the adiabatic parameter ε. In other words, one expects that to any relevant band, which is uniformly separated from the remainder of the spectrum, corresponds an orthogonal projector $\Pi^\varepsilon \in \mathcal{B}(\mathcal{H})$ so that the subspace $\mathrm{Ran}\Pi^\varepsilon \subset \mathcal{H}$ is almost invariant under the unitary evolution induced by H^ε, in the sense that[4]

$$(1 - \Pi^\varepsilon)e^{iH^\varepsilon t/\varepsilon}\Pi^\varepsilon = \mathcal{O}_0(\varepsilon^\infty). \tag{1.10}$$

[2]In Sec. 2.4.4 we will show, by exploiting a method due to Howland, that (1.9) fits in the more general framework of space-adiabatic theory.

[3]The reader should refer to the specific sections for precise mathematical statements. The only purpose of this scheme is to give to the reader an Ariadne's thread to guide him in the main body of the thesis.

[4]The meaning of the symbol $\mathcal{O}_0(\varepsilon^\infty)$ is explained in Appendix A.

For example, in the case of the Dirac electron, the band structure reduces to two twofold degenerate eigenvalues $E_\pm(q,p) = \pm\sqrt{(p - eA(q))^2 + m_e^2} + eV(q)$ separated by an energy gap $\Delta \geq 2m_e c^2$. When the external potentials are slowly varying one expects, from the physical viewpoint, that transitions from the "electronic band" E_+ to the "positronic band" E_- are forbidden to any order in ε (although *exponentially small* transitions are still possible). Then one expects that there exist two projectors $\Pi^\varepsilon_\pm$ which satisfy (1.10) and which physically correspond to electronic, resp. positronic, states.

Coming back to the general theory, it is moreover interesting to prove, as we shall do, that the operator Π^ε is $\mathcal{O}(\varepsilon^\infty)$-close to a pseudodifferential operator $\hat{\pi}$ and to give an algorithm which allows to compute the the asymptotic expansion of its symbol $\pi \asymp \sum_j \varepsilon^j \pi_j$ to any given order in ε. The existence of almost invariant subspaces will be discussed in detail in Sec. 2.2 and in Sec. 6.3.1 for the case of the Bloch electron.

B. Intertwining unitaries. The second goal of space-adiabatic theory is to study the **intraband dynamics**, i.e. the dynamics inside the almost invariant subspace $\mathrm{Ran}\Pi^\varepsilon$. Since the almost invariant subspace is ε-dependent and not easily accessible, it is convenient to map the dynamics into a fixed ε-independent subspace. It is then important to show that there exist a unitary operator $U \in \mathcal{B}(\mathcal{H})$ such that

$$U^* \Pi^\varepsilon U = \Pi_{\mathrm{ref}}, \tag{1.11}$$

where Π_{ref} is an a priori fixed and ε-independent orthogonal projector. At this point there is a certain degree of arbitrariness in the choice of Π_{ref} and U. The existence of intertwining unitaries is discussed in Sec. 2.3 and in Sec. 6.3.2 in the case of the Bloch electron.

C. Effective hamiltonian. Finally we are interested in an explicit description of the intraband dynamics, as represented in the reference Hilbert space $\mathcal{K}_{\mathrm{ref}} := \mathrm{Ran}\Pi_{\mathrm{ref}}$. In order to do that we will show that there exist a pseudodiffential operator $\widehat{h}_{\mathrm{eff}}$ which approximates the true intraband dynamics, in the sense that

$$(e^{-iH^\varepsilon t} - U\, e^{-i\widehat{h}_{\mathrm{eff}} t}\, U^*)\Pi^\varepsilon = \mathcal{O}_0(\varepsilon^\infty(1 + |t|)), \tag{1.12}$$

or a stronger property, holds true. The operator $\widehat{h}_{\mathrm{eff}}$ will be called the **effective hamiltonian** for the dynamics inside the relevant band. Moreover we will exhibit an algorithm which allows to compute, at least in principle, the asymptotic expansion of the symbol $h_{\mathrm{eff}} \asymp \sum_j \varepsilon^j h_j$ to any order in ε. This procedure, baptized **space-adiabatic perturbation theory** in [PST$_1$], is

crucial in order to obtain from the theory physically relevant information, to be compared with experiments. This topic will be covered in detail in Sec. 2.4 and in Sec. 6.3.3 in the case of the Bloch electron.

D. Dynamics of observables. The ultimate goal of any physical theory is to formulate predictions on experimentally measurable quantities. In this spirit we will discuss how to obtain from the previous construction, by using the well-known Egorov theorem, an estimate on the expectation value of the relevant quantum observables on states which initially belong to the almost invariant subspace $\mathrm{Ran}\Pi^\varepsilon$. This is the only step in which the semiclassical limit is performed. This topic will be discussed in detail in Sec. 2.5 and in Sec. 6.3.5.

In the following chapters this scheme will be performed in many relevant cases, according to the following **plan**. In Ch. 2 it is treated the abstract case of a $\mathcal{B}(\mathcal{H}_\mathrm{f})$-valued principal symbol $H(q,p)$, defined over the phase space $T^*X \cong \mathbb{R}^{2d}$, whose spectrum contains a relevant band which satisfies a global gap condition (see Condition $(\mathrm{Gap})_\sigma$). A method to extend this theory to the case of *unbounded*-operator-valued symbols and/or to situations in which only a *local* gap condition is fulfilled is outlined in Sec. ???. With this extension the theory covers the case of molecular hamiltonians (Sec.), the Pauli equation and the Dirac equation (Ch. 3). Moreover, by using the extended space formalism [Ho], the time-adiabatic approach is reconsidered as a special case of the space-adiabatic approach, and usual results recovered, see Sec. 2.4.4. The application to the Pauli-Fierz model is sketched, at a premathematical level, in Ch. 4. A rigorous treatement is possible, but it will be given elsewhere. Finally, the application to the case of the Bloch electron (Ex.4) requires a major additional effort, for two main reason:

- in the case of the Bloch electron the classical phase space is given by the cotangent bundle of a torus, $T^*X \cong \mathbb{T}^d \times \mathbb{R}^d$, and so an (operator-valued) Weyl calculus over the torus must be developed, as is done in Ch. 5.

- the symbol takes values in a space of unbounded operators, with constant domain $\mathcal{D}$, and so a suitable Weyl calculus for $\mathcal{B}(\mathcal{D},\mathcal{H}_\mathrm{f})$-valued symbol is needed. This is incorporated in the theory outlined in Ch. 5.

With this preparation, the application to the case of Bloch electron is possible, and it is performed in Ch. 6. The final chapter reviews open problems and future perspectives.

Chapter 2

General space-adiabatic theory

The results appearing in this Chapter and in the following one already appeared in [PST$_1$] and are the fruit of a joint work with Herbert Spohn and Stefan Teufel.

In this chapter, space-adiabatic perturbation theory is developed for the case of a $\mathcal{B}(\mathcal{H}_\mathrm{f})$-valued symbol defined over the phase space $\mathbb{R}^{2d}$. All the proofs relies heavily on the Weyl quantization of operator-valued symbols, which is summarized in Appendix A for reader's convenience.

2.1 General setting and assumption

Equipped with the concepts and the terminology introduced in the Appendix A, we can state the general assumptions on which the adiabatic perturbation theory will be based in the following.

Setting. Let $\mathcal{H}_\mathrm{f}$ be a separable Hilbert space and $\mathcal{H} = L^2(\mathbb{R}^d, \mathcal{H}_\mathrm{f}) \cong L^2(\mathbb{R}^d) \otimes \mathcal{H}_\mathrm{f}$. The hamiltonian $\widehat{H}$ of the full system is given as the Weyl quantization of a semiclassical symbol $H \in S^m_\rho(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ and we assume that $\widehat{H}$ is essentially self-adjoint on $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_\mathrm{f})$. 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 the following gap condition for the principal symbol H_0 of H.

Condition (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 $\sigma(z) \backslash \sigma_\mathrm{r}(z)$ 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.

$$\operatorname{dist}(\sigma(z) \setminus \sigma_{\mathrm{r}}(z), \mathrm{I}(z)) \geq C_g \langle p \rangle^{\sigma} ; \tag{2.1}$$

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

$$\sup_{z \in \mathbb{R}^{2d}} |\gamma_+(z) - \gamma_-(z)| \leq C. \tag{2.2}$$

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 after the space-adiabatic theorem.

2.2 The almost-invariant subspace

In analogy with the usual time-adiabatic theorem of quantum mechanics, see Section 2.4.4, 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] give a proof for the Dirac equation, Martinez and Sordoni [MaSo] consider Born-Oppenheimer type hamiltonians (cf. Section 2.4.3) based on results from [So], and Nenciu and Sordoni [NeSo] sketch the general scheme and apply it to a matrix-valued Klein-Gordon type problem.

Theorem 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*

$$[\widehat{H}, \Pi] = \mathcal{O}_0(\varepsilon^\infty) \tag{2.3}$$

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* $\sigma_{\rm r}(z)$.

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 $\sigma_{\rm r}(z)$. 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 $\varepsilon \to 0$.

Remark 2. Note that the growth condition on the gap in $(\mathrm{IG})_m$ is stronger than one would expect from the analysis in [NeSo] and [Te$_2$]. Indeed, in both examples a gap which is bounded globally over phase space suffices to prove uniform adiabatic decoupling also in the presence of a hamiltonian with principal symbol increasing linearly in momentum. However, [NeSo, Te$_2$] use the special structure $H_0(q,p) = D(p) + V(q)$. This is only implicit in [NeSo], but in the general case it seems difficult to establish that $[H, \pi]_{\widetilde{\#}} \in S^0(\varepsilon)$. This is the reason why we use the symbol classes S^m_ρ with $\rho > 0$, as is done in the same context also in [BrNo]. As a consequence the somewhat stronger assumption $(\mathrm{IG})_m$ is needed.

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

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

such that $\pi_0(z)$ *is the spectral projector of* $H_0(z)$ *corresponding to* $\sigma_{\rm r}(z)$, *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 $(\mathrm{IG})_m$. 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

$$\pi^{(n)} \# \pi^{(n)} - \pi^{(n)} = \varepsilon^{n+1}\, G_{n+1} + \mathcal{O}(\varepsilon^{n+2})\,, \tag{2.4}$$

where, in particular, (2.4) 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

$$\pi_{n+1}^{\mathrm{D}} = -\pi_0\, G_{n+1}\, \pi_0 + (1 - \pi_0)\, G_{n+1}\, (1 - \pi_0)\,. \tag{2.5}$$

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 $\varepsilon^{-n-1}(\pi^{(n)} \# \pi^{(n)} - \pi^{(n)})$, $\omega^{(n)} := \pi^{(n)} + \varepsilon^{n+1}\pi_{n+1}^{\mathrm{D}}$ 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

$$[H, \omega^{(n)}]_{\#} = \varepsilon^{n+1} F_{n+1} + \mathcal{O}(\varepsilon^{n+2})\,. \tag{2.6}$$

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

$$\begin{aligned} H_0(z)\, (\pi_0(z)\pi_{n+1}(z)(1 - \pi_0(z))) - (\pi_0(z)\pi_{n+1}(z)(1 - \pi_0(z)))\, H_0(z) \\ = -\pi_0(z)\, F_{n+1}(z)\, (1 - \pi_0(z)) \end{aligned} \tag{2.7}$$

for all $z \in \mathbb{R}^{2d}$. We first show that if (2.7) has a solution $\pi_0(z)\pi_{n+1}(z)(1-\pi_0(z)) =: \pi_{n+1}^{OD1}(z)$, it is unique, i.e. that the kernel of the map $\pi_{n+1}^{OD1}(z) \mapsto [H_0(z), \pi_{n+1}^{OD1}(z)]$ restricted to $\mathrm{Ran}(1-\pi_0(z))$ 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

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

and therefore

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

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

In the special case that $\sigma_{\mathrm{r}}(z) = \{E_{\mathrm{r}}(z)\}$, (2.7) can be solved, and one finds

$$\pi_0\pi_{n+1}(1-\pi_0) = \pi_0 \, F_{n+1} \, (H_0 - E_{\mathrm{r}})^{-1} \, (1-\pi_0) \, . \tag{2.8}$$

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 (2.5) and (2.8) 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 $\sigma_{\mathrm{r}}(z) = \{E_{\mathrm{r}}(z)\}$. The latter one involves four steps at each order: [a] Evaluation of G_{n+1} as in (2.4), [b] computation of π_{n+1}^{D} as in (2.5), [c] evaluation of F_{n+1} as in (2.6), [d] computation of π_{n+1}^{OD} as in (2.8).

We now turn to the construction of π in the general case. Since the Moyal product is a local operation (it depends only on the pointwise value of the symbols and their derivatives) it suffices to construct π locally in phase space and then uniqueness will liberate us from gluing the local results together.

Let us fix a point $z_0 \in \mathbb{R}^{2d}$. From the continuity of the map $z \mapsto H_0(z)$ and the gap condition it follows that there exists a neighborhood $\mathcal{U}_{z_0}$ of z_0 such that for every $z \in \mathcal{U}_{z_0}$ the set $\sigma_{\mathrm{r}}(z)$ 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,

$$\mathrm{dist}(\Gamma(z_0), \sigma(z)) \geq \frac{1}{4} C_g \langle p \rangle^{\sigma} \qquad \text{for all } z \in \mathcal{U}_{z_0} \tag{2.9}$$

and

$$\mathrm{Radius}(\Gamma(z_0)) \leq C_{\mathrm{r}} \sup_{z \in \mathcal{U}_{z_0}} \langle p \rangle^{\sigma} \, , \tag{2.10}$$

where Radius $(\Gamma(z_0))$ is the radius of the complex circle $\Gamma = \Gamma(z_0)$. The constant C_g in (2.9) is the same as in (2.1) and the existence of a constant C_{r} *independent* of z_0 such that (2.10) 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

$$R(\zeta) \# (H - \zeta 1) = 1 = (H - \zeta 1) \# R(\zeta) \qquad \text{on } \mathcal{U}_{z_0}. \tag{2.11}$$

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 $\mathcal{B}(\mathcal{H}_{\mathrm{f}})$-sense and exists according to (2.9). By induction, suppose that $R_{(n)}(\zeta) = \sum_{j=0}^{n} \varepsilon^j R_j(\zeta)$ satisfies the first equality in (2.11) 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 (2.11) which – by the associativity of the Moyal product – implies the second one.

Equation (2.11) implies that $R(\zeta)$ satisfies the *resolvent equation*

$$R(\zeta) - R(\zeta') = (\zeta - \zeta')\; R(\zeta) \# R(\zeta') \qquad \text{on } \mathcal{U}_{z_0}. \tag{2.12}$$

From the resolvent equation it follows – by using an argument similar to the standard one in operator theory [Ka$_1$] – that the symbol $\pi = \sum_{j\geq 0} \varepsilon^j \pi_j$ defined by

$$\pi_j(z) := \frac{i}{2\pi} \int_{\Gamma} R_j(\zeta, z)\; d\zeta, \qquad z \in \mathcal{U}_{z_0}\,, \tag{2.13}$$

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 (2.13) and we obtain

$$\begin{aligned}
(\pi \# \pi)_j \;&=\; \left(\frac{i}{2\pi}\right)^2 \int_{\Gamma'} d\zeta' \int_{\Gamma} d\zeta\, (R(\zeta') \# R(\zeta))_j \qquad (2.14)\\
&=\; \left(\frac{i}{2\pi}\right)^2 \int_{\Gamma'} d\zeta' \int_{\Gamma} d\zeta\, (\zeta' - \zeta)^{-1}\, [R(\zeta') - R(\zeta)]_j \\
&=\; \frac{i}{2\pi} \int_{\Gamma} R_j(\zeta)\; d\zeta = \pi_j
\end{aligned}$$

where (2.12) has been used. The first equality in (2.14) 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 (2.11). From (2.13) 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 (2.13) it follows that for every $\gamma \in \mathbb{N}^{2d}$ one has

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

According to (2.10) we are left to prove that

$$\sup_{\zeta \in \Gamma(z_0)} \left\| \left(\partial_q^\alpha \partial_p^\beta R_j\right)(\zeta, z) \right\|_{\mathcal{B}(\mathcal{H}_{\mathrm{f}})} \leq C_{\alpha\beta j} \langle p \rangle^{-\sigma - j\rho - |\beta|\rho}, \qquad \alpha, \beta \in \mathbb{N}^d,\ j \in \mathbb{N}, \tag{2.15}$$

where $C_{\alpha\beta j}$ must *not* depend on z_0. As for R_0, we notice that according to (2.9) one has

$$\left\| (H_0(z) - \zeta 1)^{-1} \right\|_{\mathcal{B}(\mathcal{H}_{\mathrm{f}})} \leq \frac{1}{\mathrm{dist}(\zeta, \sigma(H_0(z)))} \leq \frac{4}{C_g} \langle p \rangle^{-\sigma}, \tag{2.16}$$

and moreover,

$$\begin{aligned} \left\| \nabla_p R_0(z) \right\|_{\mathcal{B}(\mathcal{H}_{\mathrm{f}})} &= \left\| -(R_0 \nabla_p H_0 R_0)(z) \right\|_{\mathcal{B}(\mathcal{H}_{\mathrm{f}})} \leq \left(\frac{4}{C_g}\right)^2 \langle p \rangle^{-2\sigma} \left\| \nabla_p H_0(z) \right\|_{\mathcal{B}(\mathcal{H}_{\mathrm{f}})} \\ &\leq C \langle p \rangle^{-2\sigma + m - \rho} = C \langle p \rangle^{-\sigma - \rho}, \end{aligned}$$

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 (2.15) follows for $j = 0$. Again by induction, assume that $R_0, \ldots, R_n$ satisfy the bound (2.15). Then, by writing out

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

and using (A.7), one concludes that $R_{n+1} = -E_{n+1} R_0$ satisfies (2.15) with $\sigma = m$. □

Step II. Quantization

First of all, by resummation (Prop. 53) 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. 48) 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 Theorem 1. ♣

Essential self-adjointness of $\widehat{H}$.
Since H is an *hermitian* symbol its Weyl quantization $\widehat{H}$ is symmetric on the invariant domain $\mathcal{S}(\mathbb{R}^d, \mathcal{B}(\mathcal{H}_{\rm f})) \subseteq \mathcal{H}$. 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 50, belongs to $S_1^0(\mathcal{B}(\mathcal{H}_\mathrm{f}))$. Moreover

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

where $S_{\pm s} \in S_1^0(\varepsilon)$, since $H \in S_1^1(\varepsilon)$ and $B_{\pm s} \in S_1^0(\varepsilon)$. After Weyl quantization we obtain that

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

the latter bound following (for s large enough) from Proposition 48 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.

2.3 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* $\mathcal{K}_\mathrm{ref} := \mathrm{Ran}\Pi_\mathrm{r}$. 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.

$$u_0(z)^* \pi_0(z)\; u_0(z) = \pi_\mathrm{r}\,. \tag{2.17}$$

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 Chapter 3 that, in the case of the Dirac equation, 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 $S^0_\rho(\mathcal{B}(\mathcal{H}_{\rm f}))$. Indeed, relation (2.17) does not imply any bound at infinity on the derivatives of u_0, as can be seen by multiplying u_0 with a highly oscillating phase. Hence we *assume* that u_0 is in $S^0_\rho(\mathcal{B}(\mathcal{H}_{\rm f}))$, 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. *Assume either $(IG)_m$ or (CG) and that there exists a $\mathcal{U}(\mathcal{H}_{\rm f})$-valued map $u_0 \in S^0_\rho(\mathcal{B}(\mathcal{H}_{\rm f}))$ which satisfies (2.17). Then there exist a unitary operator $U \in \mathcal{B}(\mathcal{H})$ such that*

$$U^* \,\Pi\, U = \Pi_{\rm r} \tag{2.18}$$

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 $\pi_{\rm r}$. 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 5. *Assume either $(IG)_m$ or (CG) and that there exists a $\mathcal{U}(\mathcal{H}_{\rm f})$-valued map $u_0 \in S^0_\rho(\mathcal{B}(\mathcal{H}_{\rm f}))$ which satisfies (2.17). Then there is a formal symbol $u = \sum_{j\geq 0} \varepsilon^j u_j$, with $u_j \in S^{-j\rho}_\rho(\mathcal{B}(\mathcal{H}_{\rm f}))$, such that*

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

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

where π is the Moyal projector constructed in Lemma 3.

Remark 6. We emphasize that – as opposed to the Moyal projector π appearing in Lemma 3 – 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 $\pi_{\rm r}$ with prescribed principal symbol u_0 are parametrized by the antihermitian Moyal symbols which are diagonal in the $\pi_{\rm r}$-splitting.

Proof of Lemma 5. 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

$$\begin{aligned} u_0^* u_{n+1} + u_{n+1}^* u_0 &= -A_{n+1}, \\ u_{n+1} u_0^* + u_0 u_{n+1}^* &= -\tilde{A}_{n+1}. \end{aligned} \tag{2.19}$$

The first equation in (2.19) 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 (2.19) 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 (2.19) 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

$$b_{n+1} = [B_{n+1}, \pi_{\mathrm{r}}], \tag{2.20}$$

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

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

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 (2.20) 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 6.

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 49, $u_0 a_{n+1} \in S^{-(n+1)\rho}_\rho$ 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. 53). Then, by Weyl quantization, one gets a bounded operator $\widehat{u} \in \mathcal{B}(\mathcal{H})$ (see Prop. 48) such that:

(i) $\widehat{u}^*\widehat{u} = 1 + \mathcal{O}_{-\infty}(\varepsilon^\infty)$ and $\widehat{u}\,\widehat{u}^* = 1 + \mathcal{O}_{-\infty}(\varepsilon^\infty)$

(ii) $\widehat{u}^*\widehat{\pi}\,\widehat{u} = \Pi_{\mathrm{r}} + \mathcal{O}_{-\infty}(\varepsilon^\infty)$.

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

$$\widetilde{U} = (\widehat{u}\,\widehat{u}^*)^{-\frac{1}{2}}\,\widehat{u}\,. \tag{2.21}$$

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 (2.21) 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 as used in [NeSo]

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

defines a unitary operator $W \in \mathcal{U}(\mathcal{H})$ such that $W^*\,\widetilde{U}^*\Pi\,\widetilde{U}\,W = \Pi_{\rm r}$ and $W = 1 + \mathcal{O}_0(\varepsilon^\infty)$. Thus by defining $U = \widetilde{U}\,W$ one obtains (2.18), with the desired properties.

Remark 7. We sketch how to prove the existence of a smooth map u_0 satisfying (2.17). Given

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

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

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

where we use the fact that there exists a unitary operator $\phi(z_0) : {\rm Ran}\pi(z_0) \to \mathcal{K}_{\rm f}$. The existence of $\phi(z_0)$ follows from the fact that the dimension of ${\rm Ran}\pi(z_0)$ 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 (2.17) holds true.

2.4 Adiabatic perturbation theory

2.4.1 The effective hamiltonian

In the previous section we constructed a unitary U on $\mathcal{H}$ which exactly intertwines the almost invariant subspace $\mathrm{Ran}\Pi$ 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

$$h = u^* \# H \# u\,. \tag{2.22}$$

Recall from Appendix A 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 8. *Under the assumptions of Theorem 4, one has that $h \in S^m_\rho(\varepsilon)$ and $\widehat{h}$ is essentially self-adjoint on $\mathcal{S}$. Furthermore*

$$[\,\widehat{h},\, \Pi_{\mathrm{r}}\,] = 0\,, \tag{2.23}$$

$$e^{-i\widehat{H}t} - \widehat{u}\, e^{-i\widehat{h}t}\, \widehat{u}^* = \mathcal{O}_0(\varepsilon^\infty|t|) \tag{2.24}$$

and

$$e^{-i\widehat{H}t} - U\, e^{-i\widehat{h}t}\, U^* = \mathcal{O}_0(\varepsilon^\infty(1+|t|))\,. \tag{2.25}$$

Proof. Since $u \in S^0_\rho(\varepsilon)$ and $H \in S^m_\rho(\varepsilon)$, the composition rule for semiclassical operators (see Prop. 51) 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 (2.23) follows.

For (2.24) 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 (2.25) follows from (2.24) using $U - \widehat{u} = \mathcal{O}_0(\varepsilon^\infty)$.

Remark 9. It might seem more natural to define the effective hamiltonian as

$$H_{\text{eff}} = U^* \, \Pi \, \widehat{H} \, \Pi \, U + U^* \, (\mathbf{1} - \Pi) \, \widehat{H} \, (\mathbf{1} - \Pi) \, U \, .$$

Clearly one should have $H_{\text{eff}} - \widehat{h} = \mathcal{O}(\varepsilon^\infty)$ in some sense. However, if $\widehat{H}$ is unbounded, this closeness does not follow in the norm of bounded operators from our results, since U need not be a semiclassical operator. As a consequence no asymptotic expansion of H_{eff} in the norm of bounded operators would be available.

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 (2.23), we can, whenever appropriate, restrict our attention to the reduced Hilbert space $\mathcal{K} = \text{Ran}\Pi_{\text{r}}$. 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 (2.24) on the almost invariant subspace we obtain

$$\begin{aligned} e^{-i\widehat{H}t}\Pi &= \widehat{u} \, e^{-i\widehat{h}t} \, \Pi_{\text{r}} \, \widehat{u}^* + \mathcal{O}_0(\varepsilon^\infty |t|) \\ &= \widehat{u}^{(n)} \, e^{-it\widehat{h}^{(n+k)}} \, \Pi_{\text{r}} \, \widehat{u}^{(n)*} + (1 + |\tau|)\mathcal{O}_0(\varepsilon^{n+1}) \, , \quad |t| \leq \varepsilon^{-k}\tau \, , \end{aligned} \tag{2.26}$$

where $\rho(n + k + 1) \geq m$ 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 (2.26) to $n = 0$ and $k = 1$, one obtains the leading order solution of the Schrödinger equation as

$$e^{-i\widehat{H}t}\Pi = \widehat{u}_0 \, e^{-i(\widehat{h}_0 + \varepsilon\widehat{h}_1)t} \, \Pi_{\text{r}} \, \widehat{u}_0^* + (1 + |\tau|)\mathcal{O}_0(\varepsilon) \, , \quad |t| \leq \varepsilon^{-1}\tau \, , \tag{2.27}$$

where $m \leq 2\rho$. Here the choice of $k = 1$ corresponds to the macroscopic or semiclassical time-scale t/ε. On this time-scale the effective dynamics $e^{-i\widehat{h}t/\varepsilon}\Pi_{\text{r}}$

on the reference subspace is expected to have a nice semiclassical limit, under suitable conditions on $\widehat{h}$.

Note that one can replace in (2.26) and analogously in (2.27) τ by $\varepsilon^{-\delta}\tau$ and obtains

$$e^{-i\widehat{H}t}\Pi = \widehat{u}^{(n)}\, e^{-i\widehat{h}^{(n+k)}}\, \Pi_{\mathrm{r}}\, \widehat{u}^{(n)*} + (1+|\tau|)\mathcal{O}_0(\varepsilon^{n+1-\delta})\,, \quad |t| \leq \varepsilon^{-(k+\delta)}\tau\,. \quad (2.28)$$

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 (2.26) and (2.27) 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. Chapter 3. On the other hand, a semiclassical expansion of the right hand side of (2.27) is straightforward in many interesting cases, as will be discussed in Section 2.5.

In parentheses we remark that the space-adiabatic approximation can be used also in the time-independent setting, i.e. to estimate spectral properties of $\widehat{H}$. If one is able to compute eigenvalues of $\widehat{h}^{(n)}$ up to errors of order $o(\varepsilon^n)$,

$$\widehat{h}^{(n)}\,\psi^{(n)} = E^{(n)}\,\psi^{(n)} + o(\varepsilon^n)\,,$$

it follows that

$$\widehat{H}\,\widehat{u}\,\psi^{(n)} = E^{(n)}\,\widehat{u}\,\psi^{(n)} + o(\varepsilon^n)\,.$$

If, in addition, one knows from some a priori arguments that $\widehat{H}$ has pure point spectrum near $E^{(n)}$, it follows that $\widehat{H}$ has an eigenvalue $o(\varepsilon^n)$-close to $E^{(n)}$. Otherwise one can at least conclude that there is a "resonance" in the sense of a quasi bound state $o(\varepsilon^n)$-close to $E^{(n)}$. We stress that no explicit knowledge of U 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.

2.4.2 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 (2.22). 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 2.3. 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 (2.22). The double Moyal product becomes rather awkward to handle, and alternatively we proceed inductively by observing that

$$H \# u - u \# h_0 = \varepsilon \, u \# h_1 + \mathcal{O}(\varepsilon^2) = \varepsilon \, u_0 \, h_1 + \mathcal{O}(\varepsilon^2) \, , \tag{2.29}$$

with the subprincipal symbol on the left hand side being

$$(H \# u - u \# h_0)_1 = H_0 u_1 + H_1 u_0 - u_1 h_0 + (H_0 \# u_0)_1 - (u_0 \# h_0)_1 \, . \tag{2.30}$$

Recall the notation $a \# b = \sum_{j=0}^{\infty} \varepsilon^j \, (a \# b)_j$ for the expansion of the Moyal product, cf. Section A. Combining (2.29) and (2.30) one obtains

$$h_1 = u_0^* \, (H_0 u_1 + H_1 u_0 - u_1 h_0 + (H_0 \# u_0)_1 - (u_0 \# h_0)_1 \,) \, . \tag{2.31}$$

The expression (2.31) further simplifies if one specializes to the case where $\sigma_{\mathrm{r}}(q,p) = \{E_{\mathrm{r}}(q,p)\}$ consists of a single eigenvalue of $H_0(q,p)$ and one projects on the relevant subspace,

$$\pi_{\mathrm{r}} h_1 \pi_{\mathrm{r}} = \pi_{\mathrm{r}} \Big(u_0^* \, H_1 \, u_0 + u_0^* (H_0 \# u_0)_1 - u_0^* (u_0 \# E_{\mathrm{r}})_1 \Big) \pi_{\mathrm{r}} \, . \tag{2.32}$$

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

$$\begin{aligned} \pi_{\mathrm{r}} h_2 \pi_{\mathrm{r}} \;=\; & \pi_{\mathrm{r}} u_0^* \Big(H_2 u_0 + H_1 u_1 - u_1 h_1 \\ & + (H_0 \# u_1)_1 + (H_1 \# u_0)_1 - (u_1 \# E_{\mathrm{r}})_1 - (u_0 \# h_1)_1 \\ & + (H_0 \# u_0)_2 - (u_0 \# E_{\mathrm{r}})_2 \Big) \pi_{\mathrm{r}} \, . \end{aligned} \tag{2.33}$$

Again, (2.33) 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 2.3.

Although (2.33) 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 (2.33) 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 2.2 and 2.3 yields

$$u_1 = u_0\Big(-\frac{i}{4}\{u_0^*, u_0\} + [u_0^*\,\pi_1^{\mathrm{OD}}\,u_0, \pi_{\mathrm{r}}] + \frac{i}{4}[(\{u_0^*, \pi_0\}u_0 + u_0^*\{\pi_0, u_0\}), \pi_{\mathrm{r}}]\Big)\,, \quad (2.34)$$

with

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

where we used that $(a\,\#\,b)_1 = -\frac{i}{2}\{a, b\}$. Recall the definition (A.8) of the Poisson bracket $\{\cdot,\cdot\}$.

To compute π_1 from the given quantities one has to use the construction explained in Section 2.2. One finds

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

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

Remark 10. Note that in the case of $\sigma_{\mathrm{r}}(q,p) = \{E_{\mathrm{r}}(q,p)\}$, the principal symbol $h_0(q,p) = E_{\mathrm{r}}(q,p)\mathbf{1}_{\mathcal{H}_{\mathrm{f}}}$ and the subprincipal symbol $h_1(q,p)$ as given by (2.32) 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$_2$], [Te$_1$].

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 7). 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 $\sigma_{\rm r}(q,p) = \{E_{\rm r}(q,p)\}$ consists of a single eigenvalue of $H_0(q,p)$ of multiplicity ℓ (including $\ell = \infty$), we obtain the $\ell \times \ell$-matrix $\pi_{\rm r}\, h^{(1)}(q,p)\, \pi_{\rm r}$ as

$$h^{(1)}_{\alpha\beta} = \langle \chi_\alpha, h^{(1)}\chi_\beta\rangle = E_{\rm r}\,\delta_{\alpha\beta} + \varepsilon\, h_{1\,\alpha\beta}\,, \tag{2.35}$$

with

$$\begin{aligned} h_{1\,\alpha\beta} &= \langle \chi_\alpha, h_1\chi_\beta\rangle = \langle \psi_\alpha, H_1\psi_\beta\rangle - \frac{i}{2}\langle \psi_\alpha, \{(H_0+E_{\rm r}),\psi_\beta\}\rangle \\ &= \langle \psi_\alpha, H_1\psi_\beta\rangle - i\langle \psi_\alpha, \{E_{\rm r},\psi_\beta\}\rangle - \frac{i}{2}\langle \psi_\alpha, \{(H_0-E_{\rm r}),\psi_\beta\}\rangle\,. \end{aligned} \tag{2.36}$$

The indices α and β are matrix-indices, both running from 1 to ℓ. Equations (2.35) and (2.36) 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 (2.35) 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 Chapter 3.3, for the Dirac equation h_1 governs the spin precession. The reason for the particular splitting of the terms in (2.36) will be discussed in Section 2.5. Here we only remark that the second term in (2.36) 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.

2.4.3 Born-Oppenheimer type hamiltonians

An instructive example to which formula (2.36) applies are Born-Oppenheimer type hamiltonians of the form

$$H_{\rm BO}(q,p) = \frac{1}{2}p^2 1_{\mathcal{H}_{\rm f}} + V(q)\,, \tag{2.37}$$

$V \in S^0(\mathcal{B}(\mathcal{H}_{\rm f}))$, with an electronic energy band $e_{\rm r}(q)$ of constant multiplicity ℓ, i.e. $V(q)\pi_0(q) = e_{\rm r}(q)\pi_0(q)$. 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 $H_{\rm BO}(q,p)$ as a function of p prevents from applying the general results directly. At this point, 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 (2.36) 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 2.5.

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

$$h_{2\,\alpha\beta} = \frac{1}{2}\sum_{\mu=1}^{\ell} A_{\alpha\mu}\cdot A_{\mu\beta} + \frac{1}{2}\langle\nabla_q\psi_\alpha, \cdot\nabla_q\psi_\beta\rangle - \langle\, p\cdot\nabla_q\psi_\alpha,\; R_0(E_{\mathrm{r}})\; p\cdot\nabla_q\psi_\beta\rangle\,. \quad (2.38)$$

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 (2.38), we shortly describe how (2.33) relates to (2.38). Since $H_1 = 0$ and $H_2 = 0$ the corresponding terms in (2.33) do not contribute. Since u_0 and π_0 are functions of q only, the second term in (2.34) is the only one contributing to u_1, and thus the third term in (2.33) also vanishes after projecting with the π_{r}'s from outside the brackets. The last two terms in (2.33) cancel each other. The seventh term in (2.33) yields the first term in (2.38) and the fourth and sixth term in (2.33) combine to the second and third term in (2.38). 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

$$\begin{aligned} h_{\mathrm{BO}\,\alpha\beta}(q,p) \;&=\; \frac{1}{2}\Big(p - \varepsilon\, A(q)\Big)^2_{\alpha\beta} + e_{\mathrm{r}}(q)\delta_{\alpha\beta} + \frac{\varepsilon^2}{2}\langle\nabla_q\psi_\alpha(q), \cdot\nabla_q\psi_\beta(q)\rangle \\ &\quad - \varepsilon^2\,\langle\, p\cdot\nabla_q\psi_\alpha(q),\; R_0(E_{\mathrm{r}})(q)\; p\cdot\nabla_q\psi_\beta(q)\rangle + \mathcal{O}(\varepsilon^3)\,, \quad (2.39) \end{aligned}$$

where the first term from (2.38) nicely completes the square to the first term in (2.39). Note that the third term on the right side of (2.39) depends on q only

and is 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, (2.39) 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 (2.39). 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 Chapter 3.

2.4.4 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

$$i\varepsilon\partial_t U^\varepsilon(t,s) = H^\varepsilon(t)U^\varepsilon(t,s)\,, \qquad s \in \mathbb{R}\,, \tag{2.40}$$

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 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_2, 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 11 (Time-adiabatic theorem). *Let $H(t)$ and $\sigma_{\rm r}(t)$ be as above.*

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

$$U(t,s)^*\,\Pi(t)\,U(t,s) = \Pi(s) + \mathcal{O}_0(\varepsilon^\infty|t-s|) \tag{2.41}$$

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 $u_0(\cdot) \in C_{\rm b}^\infty(\mathbb{R}, \mathcal{B}(\mathcal{H}))$ with $u_0^*(t)\,\pi_0(t)\,u_0(t) = \pi_0(0) =: \pi_{\rm r}$ and a family of unitaries $\mathcal{U}(\cdot) \in S^0(\varepsilon, \mathcal{B}(\mathcal{H}))$ such that*

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

(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*

$$[\,h(t),\,\pi_{\rm r}\,] = 0 \qquad \textit{for all} \qquad t \in \mathbb{R} \tag{2.42}$$

and the solution of the initial value problem

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

satisfies

$$U(t,s) = \mathcal{U}(t)\,U_{\rm eff}(t,s)\,\mathcal{U}^*(s) + \mathcal{O}_0(\varepsilon^\infty|t-s|)\,. \tag{2.43}$$

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

$$h(t) \asymp \sum_{n=0}^{\infty} \varepsilon^n \left(\sum_{j+k+l=n} u_j^*(t)\,H_k(t)\,u_l(t) + \frac{i}{2} \sum_{j+k+1=n} \big(u_j^*(t)\,\dot{u}_k(t) - \dot{u}_j^*(t)\,u_k(t)\big) \right), \tag{2.44}$$

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 $\mathrm{Ran}\pi_0(t)$, 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 (2.40) through

$$\left(e^{-i\widehat{K}\sigma}\psi\right)(t) = U(t, t-\sigma)\psi(t-\sigma)\,. \tag{2.45}$$

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 $(\mathrm{Gap})_\sigma$ with $\sigma = 0$. However, because of the simple dependence of $K(t,\eta)$ on η, the conclusion of Theorem 1 and 4 hold still true in a sense to be made precise.

Indeed, by following the proof of Lemma 3 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 $S_0^1(\varepsilon)$. 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

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

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 2.2. Together with (2.45) 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 (2.41) follows.

For $u_0(t)$ one can use for example Kato's construction [Ka$_2$] and define $u_0(t)$ as the solution of the initial value problem

$$\frac{d}{dt}u_0(t) = [\dot{\pi}_0(t), \pi_0(t)]\,u_0(t)\,, \quad u_0(0) = \mathbf{1}\,.$$

Clearly $u_0(t)$ belongs to $S^0(\mathcal{B}(\mathcal{H}))$. Notice that the same construction does not work in the multidimensional case, since the evolutions in different directions do not commute. $\mathcal{U}$ can be obtained as in Section 2.3, 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 (2.44). According to Theorem 8 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 (2.45) that

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

The pointwise statement (2.43) follows again from the continuous dependence on t of all involved expressions.

2.5 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 $\sigma_{\rm r}(q,p) = \{E_{\rm r}(q,p)\}$ consists of a single eigenvalue of $H_0(q,p)$ of necessarily constant multiplicity ℓ, the principal symbol of $\widehat{h}$ is a scalar multiple of the identity, i.e. $h_0(q,p)\pi_{\rm r} = E_{\rm r}(q,p)\mathbf{1}_{\mathcal{K}_{\rm f}}$, and a semiclassical analysis of $\widehat{h}$ can be done in a standard way. 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 $E_{\rm r}(q,p)$. This results in a generalized Egorov's theorem, see Theorem 12. We emphasize that for more general energy bands $\sigma_{\rm r}(q,p)$ one cannot expect a simple semiclassical limit, at least not in the usual sense.

2.5.1 Semiclassical analysis for matrix-valued symbols

Egorov's Theorem. For the moment, we identify $\mathcal{K}_{\rm f}$ with $\mathbb{C}^\ell$ and h with $\pi_{\rm r}\, h\, \pi_{\rm r}$, 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

$$\frac{d\,\widehat{a}(t)}{dt} = \frac{i}{\varepsilon}[\widehat{h},\, \widehat{a}(t)]\,. \tag{2.46}$$

Expanding both sides of (2.46) on the level of symbols and using $[E_{\rm r}\mathbf{1}, a_n(t)] \equiv 0$, $\mathbf{1} = \mathbf{1}_{\mathbb{C}^\ell}$, one obtains the following hierarchy of equations:

$$\begin{aligned}
\frac{d\,a_0(t)}{dt} &= \{E_{\rm r}\mathbf{1}, a_0(t)\} + i[h_1, a_0(t)] && (2.47)\\
\frac{d\,a_1(t)}{dt} &= \{E_{\rm r}\mathbf{1}, a_1(t)\} + i[h_1, a_1(t)] - \frac{1}{2}(\{h_1, a_0(t)\} - \{a_0(t), h_1\}) \\
&\quad + i[h_2, a_0(t)] && (2.48)\\
\frac{d\,a_2(t)}{dt} &= \{E_{\rm r}\mathbf{1}, a_2(t)\} + i[h_1, a_2(t)] + \dots\,. && (2.49)
\end{aligned}$$

Since $da_n(t)/dt$ does not depend on higher orders, the equations can be solved iteratively. The solution of (2.47) with initial condition $a_0(q,p,0) = a_0(q,p)$ is given through

$$a_0(q,p,t) = D^*(q,p,t)\, a_0(\Phi^t(q,p))\, D(q,p,t)\,, \tag{2.50}$$

where $\Phi^t : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is the solution flow corresponding to the scalar hamiltonian $E_{\rm r}(q,p)$. 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

$$\dot{q} = \nabla_p E_{\rm r}\,, \qquad \dot{p} = -\nabla_q E_{\rm r}$$

with initial condition (q_0,p_0). $D(q,p,t)$ is the solution of

$$\frac{\partial}{\partial t} D(q,p,t) = -\,i\, h_1(\Phi^t(q,p))\, D(q,p,t)\,. \tag{2.51}$$

with initial condition $D(q,p,0) = \mathbf{1}$. One can think of (2.51) 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 (2.51) is unitary for all $(q,p,t) \in \mathbb{R}^{2d} \times \mathbb{R}$.

To see that (2.50) is indeed the solution of (2.47), note that the mappings

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

defined through (2.50) for $t \in \mathbb{R}$, i.e.

$$(\mathcal{U}(t)\, a_0)(q,p) = D^*(q,p,t)\, a_0(\Phi^t(q,p))\, D(q,p,t)\,, \tag{2.52}$$

form a one-parameter group of linear automorphisms on the Banach space $C_{\rm b}(\mathbb{R}^{2d}, \mathcal{B}(\mathbb{C}^\ell))$, 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 (2.51) are used. Hence $\mathcal{U}(t)$ is a group and it suffices to check that (2.50) solves (2.47) 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 (2.51) implies that

$$\frac{d\varphi_t}{dt} = -\,i\, h_1(\Phi^t(q,p))\, \varphi_t\,. \tag{2.53}$$

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

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

Turning to the higher order corrections (2.48), (2.49) etc., they are of the form

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

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

$$a_n(t) = \int_0^t ds\,\mathcal{U}(t-s)\,I_n(s)\,. \tag{2.54}$$

In order to solve Equation (2.48) 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 (2.48) vanishes at all times, since, according to (2.50), $a_0(t)$ is a scalar multiple of the identity for all times. In Section 3.3 the back reaction of the spin of an electron on its translational motion will be discussed on the basis of (2.48).

We summarize the preceding discussion on Egorov's theorem.

Theorem 12 (Egorov). *Let H satisfy either $(IG)_m$ for $m \leq 1$ and $\rho = 1$ or (CG) with $\rho = 0$. Let $\sigma_{\mathrm{r}}(q,p) = \{E_{\mathrm{r}}(q,p)\}$ be an eigenvalue of $H_0(q,p)$ of finite multiplicity ℓ.*
Then the classical flow Φ^t generated by $E_{\mathrm{r}}(q,p)$ and the solution of (2.51) 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 (2.50) is a solution of (2.47) 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 $t \in [-T,T]$

$$\|a(t) - \mathcal{W}_\varepsilon(a_0(t))\| \leq \varepsilon\, C_T\,, \tag{2.55}$$

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 (2.46) rigorous, note that $E_{\mathrm{r}} = \pi_{\mathrm{r}} h_0 \pi_{\mathrm{r}} \in S^m_\rho(\mathbb{R})$ with $m \leq 1$ and thus the corresponding hamiltonian vector field is smooth and bounded. It follows by standard ODE techniques [Ro] that $\partial_t a_0(\Phi^t) \in S^0_1$ and hence also $\partial_t a_0(t) \in S^0_1$, where $a_0(t)$ is given by (2.50). 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 (2.55) follows. □

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 (2.36). 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 $\mathbb{R}^d \times \mathcal{H}_\mathrm{f}$ 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 (2.36), which we denote by

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

corresponds exactly to this parallel transport along the generalized Berry connection. More precisely, the trivial connection on the trivial bundle $\mathbb{R}^{2d} \times \mathcal{H}_\mathrm{f}$ 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

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

in the sense that a section $s(q,p)$ 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 $\dot{c}(t) = (\nabla_p E_{\mathrm{r}}, -\nabla_q E_{\mathrm{r}})^{\mathrm{T}}$, this condition becomes

$$\Big(\partial_t + i\, h_{\mathrm{Be}}(q(t), p(t))\Big) s(q(t), p(t)) = 0\,. \tag{2.56}$$

If $h_1 = h_{\mathrm{Be}}$, (2.56) is exactly Equation (2.53) 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 $h_1 = h_{\mathrm{Be}}$, 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

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

to the time-evolution of the Wigner transform

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

as

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

Transport equations for matrix-valued Wigner measures are derived in [GMMP] and applied to the Dirac equation in [Sp$_2$].

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

$$(e^{-i\widehat{h}t/\varepsilon}\psi)(x) = \int_{\mathbb{R}^d} dy\, K^\varepsilon(x,y,t)\, \psi(y)\,. \tag{2.57}$$

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

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

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 (2.57) 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

$$\partial_t\, S(x,p,t) + E_{\rm r}(x, \nabla_x S(x,p,t)) = 0\,, \tag{2.58}$$

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

$$i\partial_t a_0(x,p,t) = \mathcal{L}(x,p,t)\, a_0(x,p,t) \; + h_1(x, \nabla_x S(x,p,t))\, a_0(x,p,t)\,. \tag{2.59}$$

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 (2.47), also in (2.59) h_1 contributes as an additional rotation in the transport equation for the leading order term. Since the solution of (2.58) exists only until a caustic is reached, the approximation (2.58), (2.59) to the propagator is a short time result only. The extension to arbitrary times is a complicated task, in general [MaFe].

2.5.2 An Egorov theorem

Ultimately the goal is to approximate expectation values of observables in in the original Hilbert space $\mathcal{H} = L^2(\mathbb{R}^d, \mathcal{H}_{\rm f})$ rather than in $\mathcal{H} = L^2(\mathbb{R}^d, \mathcal{K}_{\rm f})$. 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 $\sigma_{\rm r}(q,p) = \{E_{\rm r}(q,p)\}$ the effective hamiltonian $\widehat{h}$ projected on the subspace $\mathcal{K} = {\rm Ran}\Pi_{\rm r}$ 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 $\widehat{q}_{\mathcal{H}} = x \otimes \mathbf{1}_{\mathcal{H}_{\rm f}}$ and $\widehat{p}_{\mathcal{H}} = -i\varepsilon\nabla_x \otimes \mathbf{1}_{\mathcal{H}_{\rm f}}$ be the position and momentum operators of the slow degrees of freedom acting on $\mathcal{H}$ and let $\widehat{q}_{\mathcal{K}} = x \otimes \mathbf{1}_{\mathcal{K}_{\rm f}}$ and $\widehat{p}_{\mathcal{K}} = -i\varepsilon\nabla_x \otimes \mathbf{1}_{\mathcal{K}_{\rm f}}$ be the same operators acting on

$\mathcal{K}$. Then $\widehat{q}_{\mathcal{K}} = \Pi_{\rm r} U^* \widehat{q}_{\mathcal{H}} U \Pi_{\rm r} + \mathcal{O}(\varepsilon)$ and $\widehat{p}_{\mathcal{K}} = \Pi_{\rm r} U^* \widehat{p}_{\mathcal{H}} U \Pi_{\rm r} + \mathcal{O}(\varepsilon)$, 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 $\widehat{q}_{\mathcal{K}} = \Pi_{\rm r} U^* \widehat{q}_{\mathcal{H}} U \Pi_{\rm r} + \mathcal{O}(\varepsilon^2)$.

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 13. *Let H satisfy either $(IG)_m$ with $m \leq 1$ and $\rho = 1$ or (CG) with $\rho = 0$ and let $\sigma_{\rm r}(q,p) = \{E_{\rm r}(q,p)\}$ consist of a single eigenvalue of $H_0(q,p)$ of finite multiplicity ℓ. Let $b_0 \in S^0_1(\mathcal{B}(\mathcal{H}_{\rm f}))$ 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 $a_0 := \pi_{\rm r}\, u_0^*\, b_0\, u_0\, \pi_{\rm r}$ and define $a_0(t)$ is in (2.50). Then for each $T < \infty$ there is a constant $C_T < \infty$ such that for all $t \in [-T,T]$*

$$\|(B(t) - \mathcal{W}_\varepsilon(u_0\, a_0(t)\, u_0^*))\Pi\| \leq \varepsilon\, C_T\,. \tag{2.60}$$

For $b_0 = f\, \mathbf{1}_{\mathcal{H}_{\rm f}}$, with $f \in S^0_1(\mathbb{R})$, one obtains as a special case of (2.60) that

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

Corollary 13 follows from Theorem 12 and a straightforward expansion in ε of the terms to be estimated after rotation with U.

Chapter 3

Application to the Dirac equation

3.1 Adiabatic decoupling of electrons and positrons

As pointed out in the Introduction, the Dirac equation represents the first physically relevant example in which the full power of space-adiabatic perturbation theory is needed, since the not-scalar part of the symbol depends on both the canonical variables. In order to give an estimate on the magnitude of ε in relevant applications (see Sec. 3.2), in this section the use of natural units is avoided and all the relevant constrants $(\hbar, c, \ldots)$ restored.

For reader's convenience, we recall here from the Introduction that our goal is to study the Schrödinger equation

$$i\,\varepsilon\hbar\partial_s\psi_s = \widehat{H}_{\mathrm{D}}\,\psi_s \tag{3.1}$$

for macroscopic times of order 1, i.e. $|s| = \mathcal{O}(1)$, where $\widehat{H}_{\mathrm{D}}$ is the Weyl quantization of matrix-valued symbol

$$H_{\mathrm{D}}(q,p) = c\alpha\cdot\left(p - \frac{e}{c}A(q)\right) + \beta mc^2 + eV(q) \tag{3.2}$$

defined on the phase space $T^*X \cong \mathbb{R}^6$, where now Weyl quantization is in the sense of $p \mapsto -i\varepsilon\hbar\nabla_x$, i.e. on the right hand side of (A.3) 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.

We notice that $H_{\mathrm{D}}(q,p)$ has two two-fold degenerate eigenvalues

$$E_{\pm}(q,p) = \pm cp_0(q,p) + eV(q)$$

with the corresponding eigenprojectors

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

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 $A \in C_{\rm b}^\infty(\mathbb{R}^3,\mathbb{R}^3)$ and $V \in C_{\rm b}^\infty(\mathbb{R}^3,\mathbb{R})$, one finds that $H_0 \in S_1^1$ and thus the assumptions from Section 2.2 are satisfied. In particular, $\widehat{H}_{\rm D}$ 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 $\mathcal{K}_{\rm ref} = L^2(\mathbb{R}^3,\mathbb{C}^2)$ and it is convenient to define it as the range of

$$\Pi_{\rm r} := \begin{pmatrix} \mathbf{1}_{\mathbb{C}^2} & 0 \\ 0 & 0 \end{pmatrix}$$

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 ${\rm Ran}\pi_0(q,p)$. Since the degeneracy of ${\rm Ran}\pi_0(q,p)$ 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 $H_{\rm D}(q,p)$ [FoWo, Th]. The eigenvectors $\psi_\pm(q,p)$ of the operator $e_3 \cdot S(q,p)$ in ${\rm Ran}\pi_0(q,p)$ 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 $u_0 \in S_1^0$. Of course the positron part indicated by $*$'s would be given through charge conjugation. In our construction we want to emphasize, however, that no specification is needed in order to determine the expansion of the effective electron hamiltonian $\widehat{h}_{\rm e} := \Pi_{\rm r}\widehat{h}\,\Pi_{\rm r}$ 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 $A, V \equiv 0$. 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 (2.36) yields

$$h_{\mathrm{e},1}(q,p) = -\frac{\hbar e}{2p_0(q,p)}\,\sigma\cdot\left(B(q) - \frac{p_0}{c\,(p_0(q,p)+mc)}\,v(q,p)\wedge E(q)\right) =: -\frac{\hbar}{2}\,\sigma\cdot\Omega(q,p)\,. \tag{3.3}$$

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

$$\Omega(q,p) = \frac{e}{mc}\left(\frac{1}{\gamma(q,p)}\,B(q) - \frac{1}{c\,(1+\gamma(q,p))}\,v(q,p)\wedge E(q)\right)\,. \tag{3.4}$$

We remark that the second term in (2.36), the "Berry term", does not coincide with the second term in (3.4), in contrast to the claim in [BoKe$_1$]. Indeed, the compact expression (3.4) is obtained only through cancellations in more complicated expressions coming from both terms contributing in (2.36).

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

Theorem 14. *Let $A \in C^\infty_{\mathrm{b}}(\mathbb{R}^3,\mathbb{R}^3)$ and $V \in C^\infty_{\mathrm{b}}(\mathbb{R}^3,\mathbb{R})$. Then there exist orthogonal projectors $\Pi_\pm$ with $\Pi_+ + \Pi_- = \mathbf{1}$ such that $[\widehat{H}_{\mathrm{D}},\Pi_\pm] = \mathcal{O}_0(\varepsilon^\infty)$, and there exists a unitary U and $\widehat{h} \in \mathrm{OP}S^1_1$ with*

$$\widehat{h} = \begin{pmatrix} \widehat{h}_{\mathrm{e}} & 0 \\ 0 & \widehat{h}_{\mathrm{p}} \end{pmatrix}\,, \tag{3.5}$$

such that

$$e^{-i\widehat{H}_{\mathrm{D}}t} - U\,e^{-i\widehat{h}t}\,U^* = \mathcal{O}_0(\varepsilon^\infty|t|)\,. \tag{3.6}$$

Here $\widehat{h}_{\mathrm{e}}$ and $\widehat{h}_{\mathrm{p}}$ are semiclassical operators on $L^2(\mathbb{R}^3,\mathbb{C}^2)$ with

$$h_{\mathrm{e}}(q,p,\varepsilon) \asymp E_+(q,p)\mathbf{1}_{\mathbb{C}^2} + \sum_{j=1}^{\infty}\varepsilon^j\,h_{\mathrm{e},j}(q,p) \tag{3.7}$$

and $h_{\mathrm{e},j} = \pi_{\mathrm{r}}(u^*\#H_{\mathrm{D}}\#u)_j\pi_{\mathrm{r}} \in S^{1-j}_1(\mathcal{B}(\mathbb{C}^2))$ for all $j \geq 0$, where $u \in S^0_1(\varepsilon)$ is constructed as in Section 2.3. In particular, $h_{\mathrm{e},1}(q,p)$ is given by (3.3) and thus

$$\widehat{h}_{\mathrm{e}} = \left(c\sqrt{m^2c^2 + (-i\varepsilon\hbar\nabla - \frac{e}{c}A(x))^2} + eV(q)\right)\mathbf{1}_{\mathbb{C}^2} - \varepsilon\,\frac{\hbar}{2}\,\sigma\cdot\widehat{\Omega(q,p)} + \mathcal{O}_0(\varepsilon^2)\,. \tag{3.8}$$

Analogous results hold for h_{p}. The errors in (3.6) and (3.8) 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 (3.8) the giromagnetic ratio of the electron is $g = 2$. 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].

3.2 How small is ε?

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 (2.36) 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

$$\varepsilon(q,p) := \frac{\|\,\pi_{\mathrm{r}}\,h_1(q,p)\,\pi_{\mathrm{r}}\,\|}{\Delta E(q,p)} \approx \frac{\hbar\,|\nabla_p E_{\mathrm{r}}(q,p)|\,|\nabla_q E_{\mathrm{r}}(q,p)|}{\left(\Delta E(q,p)\right)^2}\,. \tag{3.9}$$

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 (3.9) yields

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

The electric field strength E in the laboratory devices hardly exceeds 10^7V/m, which would correspond to $\varepsilon_E \leq 10^{-10}$, and the magnetic field strength B reaches at most 10T yielding $\varepsilon_B \leq 10^{-8}$. 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 (2.26) and (2.28). 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.

3.3 The semiclassical limit and the BMT equation

Equipped with $h_{\mathrm{e},0}$ and $h_{\mathrm{e},1}$ we can apply the general results of Section 2.5 on the semiclassical limit to the Dirac equation. Let $\Phi_\pm^t$ be the hamiltonian flows generated by $E_\pm(q,p)$ on phase space $\mathbb{R}^6$ and let $\widehat{B} = \widehat{b}\,\mathbf{1}$, $b \in S_1^0(\mathbb{R})$, be a semiclassical observable in the unrotated Hilbert space which does not depend on spin. From Corollary 13 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 V 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 (3.8) 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 12. For each $T < \infty$ there is a constant $C_T < \infty$ such that for $t \in [-T,T]$

$$\| \sigma(t) - \widehat{\sigma_0(t)} \| \leq \varepsilon\, C_T\,, \tag{3.10}$$

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

$$\frac{\partial\, \sigma_{0k}(q,p,t)}{\partial t} = -\frac{i}{2} \Big[\sigma \cdot \Omega(\Phi_+^t(q,p)),\, \sigma_{0k}(q,p,t) \Big] \tag{3.11}$$

with initial condition $\sigma_{0k}(q,p,0) = \sigma_k$. This follows from the Equations (2.50) and (2.51) by setting $\sigma_{0k}(q,p,t) = D^*(q,p,t)\,\sigma_k\,D(q,p,t)$.

To solve Equation (3.11) 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

$$\frac{\partial\, s_k(q,p,t)}{\partial t} = -\,s_k(q,p,t)\,\wedge\,\Omega(\Phi_+^t(q,p))\,. \tag{3.12}$$

(3.12) 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 2.5, 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 $\widehat{H}_{\rm D}$ and $U^*\,\widehat{H}_{\rm D}\,U$ are isospectral and since (3.6) holds, a trace formula for the eigenvalue statistics of $\widehat{H}_{\rm D}$ could as well be derived from the semiclassical propagator of $\widehat{h} = \widehat{h}_{\rm e}\otimes\mathbf{1} + \mathbf{1}\otimes\widehat{h}_{\rm p}$. As argued in Section 2.5, the latter is somewhat easier to obtain. In [GMMP, Sp$_2$] 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 $h_{\rm e,2}$, according to (2.48) 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 (2.47), will remain scalar and thus its commutator with $h_{\rm e,2}$ in (2.48) vanishes identically for all times. The solution $b_1(t)$ of (2.48) 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 (2.48), as

the solution of

$$\frac{d\,x_1(t)}{dt} = \{E_+\mathbf{1}, x_1(t)\} + i[h_{\mathrm{e},1}, x_1(t)] - \{h_{\mathrm{e},1}, x_0(t)\} \tag{3.13}$$

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

$$\{h_{\mathrm{e},1}, x_0(t)\} = -\frac{\hbar}{2}\,\sigma \cdot \{\,\Omega, x_0(t)\}\,, \tag{3.14}$$

which is not scalar and thus responsible for the splitting of trajectories of electrons with distinct spin orientation. Hence, as in (2.54),

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

where $\mathcal{U}(t)$ is the "classical flow" defined through (2.52).

Without claim of rigor, we observe in (3.4) 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

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

and thus according to (3.13), (3.14) 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.

Chapter 4

Application to non-relativistic QED

The results appearing in this Chapter already appeared in [PST$_2$] and are the fruit of a joint work with Herbert Spohn and Stefan Teufel.

4.1 Introduction to the Pauli-Fierz model

A mathematically rigorous formulation of Quantum Electro Dynamics is one of the most outstanding challenges for mathematical physicist of the present century. However, especially in the realm of quantum optics, there are many measurable physical effects which are related to the quantized electromagnetic field but which involve only a *finite and constant* number of electrons, since at this energy scale the probability of pair production or annichilation is negligible.

It is then of interest a mathematically rigorous model for a system in which a finite number of electrons interact with the quantized self-generated electromagnetic field and, eventually, with the external electromagnetic field generated by the experimental setup, regarded as a classical field. This model is known as the Pauli-Fierz model or the non-relativistic QED and can be regarded, in a sense, as a rigorous description of the N-electrons sector of QED. A complete list of references to the wide literature on this model is beyond the scope of this thesis, so we simply refer to [Sp] and references therein.

For sake of a simple exposition, we introduce the model in the case of a single electron, but the generalization to any finite number of electrons is straightforward. The Hilbert space for the model is $\mathcal{H} = \mathcal{H}_{\rm el} \otimes \mathcal{F}_{\rm b}$ where $\mathcal{H}_{\rm el} = L^2(\mathbb{R}^d) \otimes \mathbb{C}^2$ corresponds to the electron states and

$$\mathcal{F}_{\rm b} = \bigoplus_{n\in\mathbb{N}} S_n (L^2(\mathbb{R}^d) \otimes \mathbb{C}^2)^{\otimes n}, \tag{4.1}$$

with S_n the symmetrizer, is the bosonic Fock space, corresponding to the electromagnetic field. An element of $\mathcal{F}_\mathrm{b}$ is a sequence $\Psi = (\psi^{(0)}, \psi^{(1)}, \ldots)$ such that $\psi^{(n)} \in (L^2(\mathbb{R}^d) \otimes \mathbb{C}^2)^{\otimes n}$ and $\|\Psi\|^2 = \sum_{n\in\mathbb{N}} \|\psi^{(n)}\|^2 < +\infty$.

As for the hamiltonian operator, we introduce it by using physics's notation, specializing to the case $d = 3$. The translation in mathematical language will follow. First we introduce the annichilation operators $a(k, \lambda)$, acting on $\mathcal{F}_b$, where $k \in \mathbb{R}^d$ corresponds to the wave number and λ to the elicity of the photon. They satisfy the canonical commutation relations

$$[a(k, \lambda), a(k', \lambda')] = \delta(k - k')\delta_{\lambda,\lambda'}. \tag{4.2}$$

The hamiltonian for the free electromagnetic field is given, in natural units $\hbar = 1 = c$, by

$$H_\mathrm{f} = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \omega(k) a^*(k, \lambda) a(k, \lambda) dk \tag{4.3}$$

with dispersion relation $\omega(k) = \sqrt{k^2 + m_\mathrm{ph}^2}$. The need to introduce a non-zero photon mass m_ph will be discussed later on.

The electron is minimally coupled to the electromagnetic field through the transversal self-generated electromagnetic field $A(x)$. To assure transversality one introduces the standard *dreibein* $e_1(k), e_2(k), \frac{k}{|k|}$ so that

$$A(x) = (2\pi)^{-3/2} \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \frac{1}{\sqrt{\omega(k)}} e_\lambda(k) \, (e^{ik\cdot x} a(k, \lambda) + e^{-ik\cdot x} a^*(k, \lambda)) dk \tag{4.4}$$

The simplicity of (4.4) should not hidden the fact that $A(x)$ is an operator-valued distribution, therefore a very untractable mathematical object. To get an unbounded operator acting on $\mathcal{H}$, we smoothen it over a form factor ρ, which in the corresponding classical theory would be the charge distribution. Therefore we introduce

$$A_\rho(x) = \int_{\mathbb{R}^d} \rho(x - y) A(y) dy \tag{4.5}$$

and we assume that ρ is spherically symmetric, smooth, rapidly decreasing and normalized as $\int_{\mathbb{R}^3} \rho(x) dx = 1$.

Equipped with this terminology, we introduce the Pauli-Fierz operator for a free self-interacting electron as

$$H_0 = \frac{1}{2m} (\sigma \cdot (-i\nabla_x \otimes 1 - eA_\rho(x)))^2 + 1 \otimes H_\mathrm{f} \tag{4.6}$$

acting on $\mathcal{H} = \mathcal{H}_\mathrm{el} \otimes \mathcal{F}_\mathrm{b}$, where σ denotes the vector of Pauli matrices and x the position operator in $L^2(\mathbb{R}^3)$. The hamiltonian (4.6) describes an electron interacting with the self-generated electromagnetic field. If the interaction with external

slowly varying electromagnetic potentials is included, then the hamiltonian reads

$$H^{\varepsilon}_{\mathrm{PF}} = \frac{1}{2m}(\sigma \cdot (-i\nabla_x \otimes 1 - eA_\rho(x) - eA_{\mathrm{ex}}(\varepsilon x))^2 + 1 \otimes H_{\mathrm{f}} + V_{\mathrm{ex}}(\varepsilon x) \qquad (4.7)$$

where, as usual, the adiabatic parameter $\varepsilon \ll 1$ controls the scale of space-variation of the potentials $A_{\mathrm{ex}}(\varepsilon x), V_{\mathrm{ex}}(\varepsilon x)$.

4.2 Effective dynamics for the Pauli-Fierz electron

From (4.7) it is not clear at all that the Pauli-Fierz model fits into the general scheme of space-adiabatic perturbation theory. Indeed, a suitable unitary transformation is needed.

First of all one notices that the free hamiltonian (4.6) is invariant under translations jointly of the electron and the photons. Therefore, the total momentum

$$P = P_{\mathrm{el}} \otimes 1 + 1 \otimes P_{\mathrm{f}}, \qquad P_{\mathrm{f}} = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} k a^*(k,\lambda) a(k,\lambda) dk, \qquad (4.8)$$

is conserved, $[H_0, P] = 0$. Indeed, following [TeSp], this can be seen more clearly in two steps. First one rewrites the hamiltonian (4.6) in the representation in which P_{el} is diagonal, getting

$$H_0 = \frac{1}{2m}(\sigma \cdot (p_{\mathrm{el}} \otimes 1 - eA_\rho(i\nabla_{p_{\mathrm{el}}})))^2 + 1 \otimes H_{\mathrm{f}}. \qquad (4.9)$$

Then, by the unitary transformation T, defined by

$$(T\Psi)^{(n)}(p, k_1, \ldots, k_n) = \psi^{(n)}(p - \sum_{i=1}^{n} k_i, k_1, \ldots, k_n), \qquad (4.10)$$

one transforms it to the representation in which the total momentum P is diagonal. The transformed hamiltonian $T^* H_0 T$, still denoted by H_0, is given by

$$H_0 = \frac{1}{2m}(\sigma \cdot (p - P_{\mathrm{f}} - eA_\rho(0)))^2 + H_{\mathrm{f}}. \qquad (4.11)$$

which clearly commutes with multiplication by p. As a consequence H_0 is an operator fibred over $\sigma(P) = \mathbb{R}^3$, i.e.

$$\mathcal{H} = \int_{\mathbb{R}^3}^{\oplus} \mathcal{H}_p dp \qquad H_0 = \int_{\mathbb{R}^3}^{\oplus} H_0(p) dp \qquad (4.12)$$

where the fibers $\mathcal{H}_p$ are naturally isomorphic to $\mathcal{H}_{\rm f} := \mathbb{C}^2 \otimes \mathcal{F}_{\rm b}$.

Performing the same transformation on the hamiltonian (4.7) one gets

$$H^{\varepsilon}_{\rm PF} = \frac{1}{2m}(\sigma \cdot (p - P_{\rm f} - eA_{\rho}(0) - eA_{\rm ex}(i\varepsilon\nabla_p)))^2 + H_{\rm f} + eV_{\rm ex}(i\varepsilon\nabla_p). \qquad (4.13)$$

Clearly (4.13) is not a fibred operator. However, from the representation (4.13) it is clear that the Pauli-Fierz hamiltonian $H^{\varepsilon}_{\rm PF}$ can be regarded as the ε-Weyl quantization of the operator-valued symbol

$$H_{\rm PF}(q,p) = \frac{1}{2m}(\sigma \cdot (p - P_{\rm f} - eA_{\rho}(0) - eA_{\rm ex}(q)))^2 + H_{\rm f} + eV_{\rm ex}(q), \qquad (4.14)$$

where Weyl quantization should be intended in the sense $p \mapsto p$ and $q \mapsto i\varepsilon\nabla_p$. The symbol (4.14), which takes values in the space of unbounded operators over $\mathcal{H}_{\rm f}$, can be rewritten as

$$H_{\rm PF}(q,p) = \frac{1}{2m}(p - P_{\rm f} - eA_{\rho}(0) - eA_{\rm ex}(q))^2 + H_{\rm f} + eV_{\rm ex}(q) - \frac{1}{2}e(B_{\rho}(0) + \varepsilon B_{\rm ex}(q)) \cdot \sigma. \qquad (4.15)$$

Notice that this symbol has a rather particular structure, which we abbreviate as

$$H_{\rm PF}(q,p) = D(p - eA_{\rm ex}(q)) + eV_{\rm ex}(q)1_{\mathcal{H}_{\rm f}} - \frac{1}{2}e\varepsilon B_{\rm ex}(q). \qquad (4.16)$$

Therefore, any information on the band structure can be deduced from the knowledge of the function $D(p)$, which is the same for the interacting hamiltonian (4.7) and for the free hamiltonian (4.6).

The physically relevant band consists of the eigenvalue of lowest energy, for any fixed (q,p). By the special structure (4.16), the eigenvectors of lowest energy $\psi_{\alpha}(q,p)$ (here α is a degeneracy index) are characterized by the property $D(p)\psi_{\alpha}(p) = E_0(p)\psi_{\alpha}(p)$ which involves only the free hamiltonian. Therefore we can use the results proved in [HiSp]: by spin degeneracy, the ground state subspace turns out to have dimension 2, and the eigenvalue $E_0(p)$ is isolated from the rest of the spectrum for $|p| \leq p_c$, provided that the interaction is cut off in in the infrared. Indeed, physically one expects that states with $|p| \geq p_c$ decay through Cerenkov radiation.

It is now evident that the general scheme developed in Ch. 2 can be applied to the Pauli-Fierz model, apart for the problem related to the presence of *unbounded*-operator valued symbols and to the fact that the gap condition is only *locally* satisfied. Although these problems can be cured, a detailed and rigorous treatment will be given elsewhere. Here we simply apply formally the scheme outlined in Ch. 2.

The last step missing to apply space-adiabatic theory consists in a choice for the fundamental unitary u_0 or, equivalently, a choice of a basis in the lowest

energy eigenspace. It is convenient to choose a basis $\{\psi_+(p), \psi_-(p)\}$ such that $\psi_+(p)$ corresponds to the electron pointing along the positive z direction. For this purpose, one notices that the total angular momentum J in the direction p is conserved, i.e. $[D(p), p \cdot J] = 0$. With this choice of the basis, the effective hamiltonian is given by

$$\begin{aligned} h_{\text{eff}}(q,p)_{\alpha,\beta} &= (E_0(p - eA_{\text{ex}}(q)) + eV_{\text{ex}}(q))\delta_{\alpha,\beta} \\ &- \frac{1}{2}\varepsilon e\{B_{\text{ex}}(q) \cdot \langle \psi_\alpha(\tilde{p}), \sigma\psi_\beta(\tilde{p})\rangle_{\mathcal{H}_{\text{f}}} \\ &+ (\nabla V_{\text{ex}}(q) - v(\tilde{p}) \wedge B_{\text{ex}}(q)) \cdot \langle \psi_\alpha(\tilde{p}), i\nabla\psi_\beta(\tilde{p})\rangle_{\mathcal{H}_{\text{f}}} \\ &+ B_{\text{ex}}(q) \cdot \langle \psi_\alpha(\tilde{p}), \nabla D(\tilde{p}) \wedge i\nabla\psi_\beta(\tilde{p})\rangle_{\mathcal{H}_{\text{f}}}\} + \mathcal{O}(\varepsilon^2) \end{aligned}$$

where $\alpha, \beta \in \{\pm\}$ are degeneracy indexes, $\tilde{p} = p - eA_{\text{ex}}(q)$ and $v(\tilde{p}) = \nabla E_0(\tilde{p})$.

The zeroth-order term in (4.17) corresponds to the analogous of Peierl's substitution, i.e. the replacement of the free kinetic energy $E_{\text{free}}(p) = \frac{1}{2}p^2$ with the modified kinetic energy $E_0(p)$, which takes into account the effect of the "photon cloud" around the electron. The first-order term contains the spin-dynamics.

4.3 The g-factor for the Pauli-Fierz electron

An interesting consequence of (4.17) is that it allows us to obtain a non-perturbative definition of the giromagnetic ratio (the g-factor) of the electron in the Pauli-Fierz model.

The experimental situation we are referring to consists of an electron moving in a constant magnetic field B. One expects that the electron follows a circular orbit with frequency ω_c. On the other hand, one measures the spin precession, with frequency ω_s. By definition, the experimental g-factor is given by

$$g = 2\omega_s/\omega_c \tag{4.17}$$

where the experimentally measured values of ω_c and ω_s appear.

What about the theoretical predictions of the Pauli-Fierz model? We consider the effective hamiltonian (4.17) with $B_{\text{ex}}(q) = B$, $V_{\text{ex}}(q) \equiv 0$ and small velocities $v = \nabla E_0(\tilde{p})$, which means $\tilde{p} \simeq 0$ in good approximation. Moreover in this section we reintroduce the bare mass m of the electron, the velocity of light c and the Planck constant $\hbar$. As far as the translational motion is concerned, by considering the semiclassical limit on (4.17) we obtain that, at the leading order in ε, the trajectory satisfies the equation

$$M_{\text{eff}}\ddot{q} = \frac{e}{c}q \wedge B$$

with effective mass $M_{\text{eff}} = (E_0''(0))^{-1}$. Moreover, by the rotational invariance of the Pauli-Fierz model, the effective mass M_{eff} is a multiple of the identity, denoted as m_{eff}. Therefore, the prediction on the cyclotron frequency is $\omega_c = e/m_{\text{eff}}c$. In other words, the only effect of the self-generated electromagnetic field on the translational motion consists in a redefinition of the electron mass.

As for the spin, from (4.17) we get

$$h_{\text{eff}} = -\frac{e\hbar}{2m} B(q) \cdot (\langle \psi_\alpha(0), \sigma\psi_\beta(0)\rangle_{\mathcal{H}_{\text{f}}} + i\langle \psi_\alpha(0), \nabla D(0) \wedge \nabla\psi_\beta(0)\rangle_{\mathcal{H}_{\text{f}}}). \quad (4.18)$$

The previous hamiltonian implicitly defines the frequency ω_s, yielding a non perturbative definition of the g-factor in the Pauli-Fierz model.

The matrix elements in (4.18) and for $E''(0)$ are not available as closed formulae. In order to have numerical predictions, the only possibility is a perturbative expansion in e around $e = 0$, or equivalently in the fine-structure constant $\alpha := 4\pi e^2$. To second order in e and after removing the infrared cut off one obtains

$$g = 2(1 + \frac{8}{3}\frac{\alpha}{2\pi} + \mathcal{O}(\alpha^2)). \quad (4.19)$$

This result is in agreement with [GrKa], in which the static perturbation theory for the Zeeman splitting. We emphasize that, as opposed to other approaches, the approach in this section gives a dynamical and non perturbative definition of the giromagnetic ratio. A perturbative approach has been used only as a last step, in order to obtain a numerical prediction.

Chapter 5

Interlude: operator-valued Weyl calculus over the torus

The results appearing in this Chapter and the following one will appear in a forthcoming paper [PST$_3$] and are the fruit of a joint work with Herbert Spohn and Stefan Teufel.

The first act in the drama of space-adiabatic perturbation theory is concluded: we developed a general theory in Ch. 2 and we applied it to molecular hamiltonians, to the Dirac equation and finally to the Pauli-Fierz model. Before we start with the second act, namely the application of this scheme to the Bloch electron, a mathematical interlude is due, in order to develop the needed mathematical tools.[1]

Indeed, in order to apply the general scheme to the Bloch electron, two main obstacles should be overwhelmed. First, one should face the problems related to the appearance of *unbounded*-operator-valued symbols. Luckily, we have to face the case of unbounded operators with a common dense domain $\mathcal{D}$, and so they can be regarded as elements of $\mathcal{B}(\mathcal{D}, \mathcal{H}_\mathrm{f})$ when $\mathcal{D}$ is equipped with a suitable inner product. Second, and more important, in the case of the Bloch electron the classical phase space is given by $T^*X \cong \mathbb{T}^d \times \mathbb{R}^2$. This means that one should consider the Weyl quantization of (operator-valued) functions over the cotangent bundle of the torus. Moreover, it will be clear in Ch. 6 that this is not enough: we need, more generally, a Weyl quantization scheme for morphism of a specific Hilbert space bundle over the cotangent bundle of the torus. From another point of view, these morphisms can be regarded as usual operator-valued symbols over $\mathbb{R}^{2d}$ which are τ-equivariant (see Definition 21 below) with respect to some representation τ of the group of lattice translations. Their quantization

[1] The reader interested mainly in physical applications can skip this Chapter at a first reading.

acts on a space of locally-L^2 sections of a specific Hilbert space bundle over the cotangent bundle of the torus.

It is worthwhile to mention that in the literature there are many schemes to generalize Weyl quantization to (scalar) functions defined over the torus or even over a general riemannian manifold. However, no one of them retain the full computational power of the Weyl calculus, namely a suitable generalization of the *Weyl product* which allows to compute the symbol of the product of two pseudors from the knowledge of the symbols of the factors. For this reason in [PST$_3$] we had to developed the theory by ourselves. Similar ideas were used by Gérard and Nier [GeNi] in the case of (scalar-valued) functions over $\mathbb{T}^d \times \mathbb{R}^d$, i.e. in the case of a trivial bundle. We recover their results in this case.

We start with fixing some notation and recalling a few facts from from the usual pseudodifferential and semiclassical calculus for operator valued symbols, which complements the review given in the Appendix A. For an extended exposition of the general calculus for scalar symbols we refer, for example, to [DiSj] and for an explicit discussion of the operator valued case to [GMS].

Definition 15. *A function $w : \mathbb{R}^{2d} \to [0, +\infty)$ is said to be an* ***order function*** *if there exist $C_0 > 0$ and $N_0 > 0$ such that $w(x) \leq C_0 \, \langle x - y \rangle^{N_0} \, w(y)$ for every $x, y \in \mathbb{R}^{2d}$.*

Let w be an order function and $\mathcal{H}_1$ and $\mathcal{H}_2$ separable Hilbert spaces.

Definition 16. *A function $A \in C^\infty(\mathbb{R}^{2d}, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ belongs to the symbol class $S(w, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ if for every $\alpha, \beta \in \mathbb{N}^d$ there exists a positive constant $C_{\alpha,\beta}$ such that*

$$\left\| (\partial_q^\alpha \partial_p^\beta A)(q,p) \right\|_{\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)} \leq C_{\alpha,\beta} \; w(q,p) \tag{5.1}$$

for every $q, p \in \mathbb{R}^d$.

Definition 17. *A map $A : [0, \varepsilon_0) \to S(w, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)), \varepsilon \mapsto A_\varepsilon$ is called a* ***semiclassical symbol*** *of order w if (5.1) holds uniformly for $\varepsilon \in [0, \varepsilon_0)$. The space of semiclassical symbols of order w is denoted as $S^\varepsilon(w, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$.*

The spaces $S(w, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ and $S^\varepsilon(w, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ are Fréchet spaces and a family of seminorms is given, for example, by the minimal constants $C_{\alpha,\beta}$ satisfying (5.1).

Definition 18. *A formal power series $A = \sum_{j=0}^\infty \varepsilon^j \, A_j$ with coefficients $\{A_j\}_{j \in \mathbb{N}} \subset S(w, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ is called a* **formal symbol**. *If a semiclassical symbol $A_\varepsilon \in S^\varepsilon(w, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ satisfies*

$$\varepsilon^{-n} \left(A_\varepsilon - \sum_{j=0}^{n-1} \varepsilon^j A_j \right) \in S^\varepsilon(w, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$$

for all $n \in \mathbb{N}$, then A_ε is said to be asymptotically equivalent to the formal symbol A and one writes

$$A_\varepsilon \asymp \sum_{j=0}^{\infty} \varepsilon^j A_j \,.$$

The space of formal symbols is denoted as $M^\varepsilon(w, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$.

If A_ε is asymptotically equivalent to the series in which $A_j = 0$ for every $j \in \mathbb{N}$, we write $A_\varepsilon = \mathcal{O}(\varepsilon^\infty)$ in $S^\varepsilon(w, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$.

The Weyl product of two symbols is, at first formally, given as

$$(A_\varepsilon \tilde{\#} B_\varepsilon)(q,p) := \exp\left(\frac{\mathrm{i}\varepsilon}{2}(\nabla_p \cdot \nabla_x - \nabla_\xi \cdot \nabla_q)\right)(A_\varepsilon(q,p)B_\varepsilon(x,\xi))|_{x=q,\xi=p}. \quad (5.2)$$

Proofs of the following two propositions for operator valued symbols can be found in the Appendix of [GMS].

Proposition 19. *Let $A_\varepsilon \in S^\varepsilon(w_1, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ and $B_\varepsilon \in S^\varepsilon(w_2, \mathcal{B}(\mathcal{H}_2, \mathcal{H}_3))$. Then $A_\varepsilon \tilde{\#} B_\varepsilon$ belongs to $S^\varepsilon(w_1 w_2, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_3))$ and the map $(A_\varepsilon, B_\varepsilon) \mapsto A_\varepsilon \tilde{\#} B_\varepsilon$ is continuous.*

The Weyl product for semiclassical symbols induces a corresponding product on the level of formal power series, called the Moyal product and denoted by $\#$.

Proposition 20. *Let $A_\varepsilon \in S^\varepsilon(w_1, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ and $B_\varepsilon \in S^\varepsilon(w_2, \mathcal{B}(\mathcal{H}_2, \mathcal{H}_3))$ such that $A_\varepsilon \asymp A \in M^\varepsilon(w_1, \mathcal{B}(\mathcal{H}_2, \mathcal{H}_3))$ and $B_\varepsilon \asymp B \in M^\varepsilon(w_2, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$. Then*

$$A_\varepsilon \tilde{\#} B_\varepsilon \asymp C =: A \# B \in M^\varepsilon(w_1 w_2, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_3)) \,.$$

After these general definitions we now introduce an operator valued Weyl calculus for τ-equivariant symbols acting on τ-equivariant functions.

Let $\Gamma \subset \mathbb{R}^d$ be a regular lattice and let

$$B := \left\{ x \in \mathbb{R}^d : x = \sum_{j=1}^{d} \alpha_j \gamma_j \text{ for } \alpha_j \in [-\tfrac{1}{2}, \tfrac{1}{2}] \right\} \quad (5.3)$$

be the corresponding centered fundamental cell. Clearly the translations on $\mathbb{R}^d$ by elements of Γ form an abelian group G isomorphic to $\mathbb{Z}^d$.

Let $\mathcal{H}$ be a separable Hilbert space and let τ be a representation of G in $\mathcal{B}^*(\mathcal{H})$, the group of invertible elements of $\mathcal{B}(\mathcal{H})$, i.e. a group homomorphism

$$\tau : G \to \mathcal{B}^*(\mathcal{H}), \qquad \gamma \mapsto \tau(\gamma) \,. \quad (5.4)$$

If more than one Hilbert space appears, then τ denotes a collection of such representations, i.e. one on each Hilbert space.

Let L_γ be the operator of translation by $\gamma \in G$ on $\mathcal{S}(\mathbb{R}^d, \mathcal{H})$, i.e. $(L_\gamma \varphi)(x) = \varphi(x - \gamma)$, and extend it by duality to distributions, i.e. for $T \in \mathcal{S}'(\mathbb{R}^d, \mathcal{H})$ let $(L_\gamma T)(\varphi) = T(L_{-\gamma}\varphi)$.

Definition 21. *A tempered distribution $T \in \mathcal{S}'(\mathbb{R}^d, \mathcal{H})$ is said to be* τ-equivariant *if*

$$L_\gamma T = \tau(\gamma) T \quad \textit{for all } \gamma \in G\,, \tag{5.5}$$

where $(\tau(\gamma)T)(\varphi) = T(\tau(\gamma)^{-1}\varphi)$ for $\varphi \in \mathcal{S}(\mathbb{R}^d, \mathcal{H})$. The subspace of τ-equivariant distributions is denoted as $\mathcal{S}'_\tau$. Analogously we define

$$\mathcal{H}_\tau = \Big\{ \psi \in L^2_{\rm loc}(\mathbb{R}^d, \mathcal{H}) : \psi(x-\gamma) = \tau(\gamma)\,\psi(x) \quad \textit{for all } \gamma \in G \Big\}\,, \tag{5.6}$$

which, equipped with the inner product

$$\langle \varphi, \psi \rangle_{\mathcal{H}_\tau} = \int_B \mathrm{d}x\, \langle \varphi(x), \psi(x) \rangle_{\mathcal{H}}\,, \tag{5.7}$$

is a Hilbert space. Clearly

$$C^\infty_\tau = \Big\{ \psi \in C^\infty(\mathbb{R}^d, \mathcal{H}) : \psi(x-\gamma) = \tau(\gamma)\,\psi(x) \quad \textit{for all } \gamma \in G \Big\}\,, \tag{5.8}$$

is a dense subspace of $\mathcal{H}_\tau$. ◇

Notice that if τ is a unitary representation, then for any $\varphi, \psi \in \mathcal{H}_\tau$ the map $x \mapsto \langle \varphi(x), \psi(x) \rangle_{\mathcal{H}}$ is periodic, since

$$\langle \varphi(x-\gamma), \psi(x-\gamma) \rangle_{\mathcal{H}} = \langle \tau(\gamma)\varphi(x), \tau(\gamma)\psi(x) \rangle_{\mathcal{H}} = \langle \varphi(x), \psi(x) \rangle_{\mathcal{H}}\,.$$

Now that we have τ-equivariant functions, we define τ-equivariant symbols.

Definition 22. *Let w be an order function. A symbol $A_\varepsilon \in S^\varepsilon(w, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ is* τ-equivariant *(more precisely (τ_1, τ_2)-equivariant), if*

$$A_\varepsilon(q-\gamma, p) = \tau_2(\gamma)\, A_\varepsilon(q,p)\, \tau_1(\gamma)^{-1} \quad \textit{for all } \gamma \in G\,.$$

The space of τ-equivariant symbols is denoted as $S^\varepsilon_\tau(w, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$. ◇

Notice that the coefficients in the asymptotic expansion of a τ-equivariant semiclassical symbol must be as well τ-equivariant, i.e. if $A_\varepsilon \asymp \sum_{j=0}^\infty \varepsilon^j A_j$, $A_\varepsilon \in S^\varepsilon_\tau(w, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$, then $A_j \in S_\tau(w, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$.

Given any τ-equivariant symbol $A \in S_\tau(w, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$, one can consider the usual Weyl quantization $\widehat{A}$, regarded as an operator acting on $\mathcal{S}'(\mathbb{R}^d, \mathcal{H}_1)$ with distributional integral kernel

$$K_A(x,y) = \frac{1}{(2\pi\varepsilon)^d} \int_{\mathbb{R}^d} A(\tfrac{1}{2}(x+y), \xi)\; e^{i\xi\cdot(x-y)/\varepsilon}\; \mathrm{d}\xi. \tag{5.9}$$

Notice that integral kernel associated to a τ-equivariant symbol A is τ-equivariant in the following sense:

$$K_A(x-\gamma, y-\gamma) = \tau_2(\gamma)\, K_A(x,y)\, \tau_1(\gamma)^{-1} \quad \text{for all } \gamma \in G\,. \tag{5.10}$$

The simple but important observation is that the space of τ-equivariant distributions is invariant under the action of quantizations of τ-equivariant symbols.

Proposition 23. *Let $A \in S_\tau(w, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$, then $\widehat{A}\, \mathcal{S}'_{\tau_1}(\mathbb{R}^d, \mathcal{H}_1) \subset \mathcal{S}'_{\tau_2}(\mathbb{R}^d, \mathcal{H}_2)$.*

Proof. Since $\widehat{A}$ maps $\mathcal{S}'(\mathbb{R}^d, \mathcal{H}_1)$ continuously into $\mathcal{S}'(\mathbb{R}^d, \mathcal{H}_2)$, we only need to show that $(L_\gamma \widehat{A} T)(\varphi) = (\tau_2(\gamma)\widehat{A}T)(\varphi)$ for all $T \in \mathcal{S}'_{\tau_1}(\mathbb{R}^d, \mathcal{H}_1)$ and $\varphi \in \mathcal{S}(\mathbb{R}^d, \mathcal{H}_2)$.

To this end notice that as acting on $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_2)$ one finds by direct computation using (5.9) that $\widehat{A^*}\, L_\gamma = L_\gamma\, (\tau_1(\gamma)^{-1})^*\, \widehat{A^*}\, \tau_2(\gamma)^*$. Indeed, let $\psi \in \mathcal{S}(\mathbb{R}^d, \mathcal{H}_2)$, then

$$\begin{aligned}
(\widehat{A^*}\, L_\gamma\, \psi)(x) &= \int_{\mathbb{R}^d} \mathrm{d}y\, K_{A^*}(x,y)\, \psi(y-\gamma) = \int_{\mathbb{R}^d} \mathrm{d}y\, K_{A^*}(x, y+\gamma)\, \psi(y) \\
&= \int_{\mathbb{R}^d} \mathrm{d}y\, (\tau_1(\gamma)^{-1})^*\, K_{A^*}(x-\gamma, y)\, \tau_2(\gamma)^*\, \psi(y) \\
&= \Big(L_\gamma\, (\tau_1(\gamma)^{-1})^*\, \widehat{A^*}\, \tau_2(\gamma)^*\, \psi\Big)(x)
\end{aligned}$$

Hence, using the fact that τ is a representation and that $L_\gamma T = \tau_1(\gamma) T$,

$$\begin{aligned}
(L_\gamma \widehat{A} T)(\varphi) &= T(\widehat{A}^*\, L_{-\gamma}\, \varphi) = T(L_{-\gamma}\, \tau_1(\gamma)^*\, \widehat{A}^*\, (\tau_2(\gamma)^{-1})^*\, \varphi) \\
&= (\tau_2(\gamma)\, \widehat{A}\, \tau_1(\gamma)^{-1}\, L_\gamma\, T)(\varphi) = (\tau_2(\gamma)\, \widehat{A}\, T)(\varphi)\,.
\end{aligned}$$

□

Next observe that τ-equivariance of symbols is preserved under the pointwise product, the Weyl product and the Moyal product.

Proposition 24. *Let $A_\varepsilon \in S^\varepsilon_\tau(w_1, \mathcal{B}(\mathcal{H}_2, \mathcal{H}_3))$ and $B_\varepsilon \in S^\varepsilon_\tau(w_2, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$, then $A_\varepsilon B_\varepsilon \in S^\varepsilon_\tau(w_1 w_2, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_3))$ and $A_\varepsilon \mathbin{\widetilde{\#}} B_\varepsilon \in S^\varepsilon_\tau(w_1 w_2, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_3))$.*

Proof. One has

$$\begin{aligned}
A_\varepsilon(q-\gamma, p) B_\varepsilon(q-\gamma, p) &= \tau_3(\gamma) A_\varepsilon(q,p) \tau_2(\gamma)^{-1} \tau_2(\gamma) B_\varepsilon(q,p) \tau_1(\gamma)^{-1} \\
&= \tau_3(\gamma) A_\varepsilon(q,p) B_\varepsilon(q,p) \tau_1(\gamma)^{-1}\,,
\end{aligned}$$

which shows $A_\varepsilon B_\varepsilon \in S^\varepsilon_\tau(w_1 w_2, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_3))$ and inserted into (5.2) yields immediately also $A_\varepsilon \mathbin{\widetilde{\#}} B_\varepsilon \in S^\varepsilon_\tau(w_1 w_2, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_3))$. □

As for the Moyal product of formal symbol, an analogous statement holds true.

A not completely obvious fact is the following variant of the Calderon-Vaillancourt theorem.

Theorem 25. *Let $A \in S_\tau(1, \mathcal{B}(\mathcal{H}))$ and τ a unitary representation, then $\widehat{A} \in \mathcal{B}(\mathcal{H}_\tau)$ and for $A_\varepsilon \in S^\varepsilon_\tau(1, \mathcal{B}(\mathcal{H}))$ we have that $\sup_{\varepsilon\in[0,\varepsilon_0)} \|\widehat{A}_\varepsilon\|_{\mathcal{B}(\mathcal{H}_\tau)} < \infty$.*

Proof. Fix $n > d/2$ and let $w(x) = \langle x\rangle^{-n}$. We consider the weighted L^2-space

$$L^2_w = \left\{\psi \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathcal{H}) : \int_{\mathbb{R}^d} \mathrm{d}x\, w(x)^2 |\psi(x)|^2 < \infty\right\}.$$

Then $\mathcal{H}_\tau \subset L^2_w$ and for any $\psi \in \mathcal{H}_\tau$ one has the norm equivalence

$$C_1 \|\psi\|_{\mathcal{H}_\tau} \leq \|\psi\|_{L^2_w} \leq C_2 \|\psi\|_{\mathcal{H}_\tau} \tag{5.11}$$

for appropriate constants $0 < C_1, C_2 < \infty$. The first inequality in (5.11) is obvious and the second one follows by exploiting τ-equivariance of ψ and unitarity of τ:

$$\begin{aligned}\|\psi\|^2_{L^2_w} &= \sum_{\gamma\in G} \int_{B+\gamma} \mathrm{d}x\, w(x)^2 \|\tau(\gamma)^{-1}\psi(x)\|^2_{\mathcal{H}} = \sum_{\gamma\in G} \int_{B+\gamma} \mathrm{d}x\, w(x)^2 \|\psi(x)\|^2_{\mathcal{H}} \\ &\leq \sum_{\gamma\in G} \sup_{x\in B+\gamma} \{w(x)^2\} \int_B \mathrm{d}x\, \|\psi(x)\|^2_{\mathcal{H}} \leq C_2 \|\psi\|_{\mathcal{H}_\tau}.\end{aligned}$$

According to (5.11) it suffices to show that $\widehat{A} \in \mathcal{B}(L^2_w)$ and to estimate the norm of $\widehat{A}_\varepsilon$ in this space.

Let $\psi \in C^\infty_\tau(\mathbb{R}^d, \mathcal{H})$, then by the general theory $\widehat{A}\psi$ is smooth as well (cf. [Fo], Corollary 2.62) and thus, according to Prop. 23, $\widehat{A}\psi \in C^\infty_\tau(\mathbb{R}^d, \mathcal{H})$. Hence we can use (5.11) and find

$$\|\widehat{A}\psi\|_{L^2_w} = \|w\widehat{A}\psi\|_{L^2} \leq \|w\widehat{A}w^{-1}\|_{\mathcal{B}(L^2)} \|w\psi\|_{L^2} = \|w\widehat{A}w^{-1}\|_{\mathcal{B}(L^2)} \|\psi\|_{L^2_w}.$$

However, by Prop. 19, we have that $w \mathbin{\widetilde{\#}} A \mathbin{\widetilde{\#}} w^{-1} \in S(1, \mathcal{B}(\mathcal{H}))$. Thus from the usual Calderon-Vaillancourt theorem it follows that

$$\|w\, \widehat{A}\, w^{-1}\|_{\mathcal{B}(L^2)} \leq C_d \| w \mathbin{\widetilde{\#}} A \mathbin{\widetilde{\#}} w^{-1}\|_{C^{2d+1}_{\mathrm{b}}(\mathbb{R}^{2d})}.$$

This shows that for $A \in S_\tau(1, \mathcal{B}(\mathcal{H}))$ we have $\widehat{A} \in \mathcal{B}(\mathcal{H}_\tau)$. Since also $w \mathbin{\widetilde{\#}} A_\varepsilon \mathbin{\widetilde{\#}} w^{-1} \in S^\varepsilon(1, \mathcal{B}(\mathcal{H}))$ for $A_\varepsilon \in S^\varepsilon_\tau(1, \mathcal{B}(\mathcal{H}))$, we conclude that

$$\sup_{\varepsilon\in[0,\varepsilon_0)} \|\widehat{A}_\varepsilon\|_{\mathcal{B}(\mathcal{H}_\tau)} < \infty \tag{5.12}$$

by the same argument. □

By essentially the same argument, one proves the following proposition involving two Hilbert spaces.

Proposition 26. *Let $A_\varepsilon \in S^\varepsilon_\tau(1, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ a (τ_1, τ_2)-equivariant symbol with both τ_1 and τ_2 unitary representations. Then $\widehat{A}_\varepsilon$ is a bounded operator from $L^2_{\tau_1}(\mathbb{R}^d, \mathcal{H}_1)$ to $L^2_{\tau_2}(\mathbb{R}^d, \mathcal{H}_2)$ and*

$$\sup_{\varepsilon \in [0, \varepsilon_0)} \|\widehat{A}_\varepsilon\|_{\mathcal{B}(L^2_{\tau_1}, L^2_{\tau_2})} < \infty. \tag{5.13}$$

Proof. We use the shorthands $L^2_{\tau_i}$ for $L^2_{\tau_i}(\mathbb{R}^d, \mathcal{B}(\mathcal{H}_i))$ and $L^2_{w_i}$ for $L^2_w(\mathbb{R}^d, \mathcal{B}(\mathcal{H}_i))$, with w as in the previous proof. By exploiting the unitarity of τ_i one gets that for any $\psi \in L^2_{\tau_i}$

$$C_1 \|\psi\|_{L^2_{\tau_i}} \leq \|\psi\|_{L^2_{w_i}} \leq C_2 \|\psi\|_{L^2_{\tau_i}}. \tag{5.14}$$

For any $\psi \in C^\infty_{\tau_1}(\mathbb{R}^d, \mathcal{H}_1)$ we know *a priori* (by combining [Fo], Corollary 2.62 and Prop.23) that $\widehat{A}_\varepsilon \psi \in C^\infty_{\tau_2}(\mathbb{R}^d, \mathcal{H}_2)$. Hence we can use (5.14) so that the problem is reduced to prove that $\widehat{A}_\varepsilon$ belongs to $\mathcal{B}(L^2_{w_1}, L^2_{w_2})$ and to estimate its norm in this space. This can be done exactly as in the previous Theorem, exploiting the fact that $w \widetilde{\#} A_\varepsilon \widetilde{\#} w^{-1} \in S^\varepsilon(1, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ for any A_ε in $S^\varepsilon_\tau(1, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$. □

Remark 27. It is clear from the proof that both the previous result still hold true under the weaker assumption that τ_1 and τ_2 are uniformly bounded, i.e.

$$\sup_{\gamma \in G} \|\tau_i(\gamma)\|_{\mathcal{B}(\mathcal{H}_i)} \leq C \qquad \forall \gamma \in G,\ i \in \{1, 2\}. \tag{5.15}$$

Finally we would also like to show that for $A \in S_\tau(w, \mathcal{B}(\mathcal{H}))$ the adjoint of $\widehat{A}$ as an operator in $\mathcal{B}(\mathcal{H}_\tau)$, denoted by $\widehat{A}^\dagger$, is given through the quantization of the pointwise adjoint, i.e. through $\widehat{A^*}$. Here it is crucial that τ is a unitary representation.

Proposition 28. *Let $S_\tau(w, \mathcal{B}(\mathcal{H}))$ with a unitary representation τ and let $\widehat{A}^\dagger$ be the adjoint of $\widehat{A} \in \mathcal{B}(\mathcal{H}_\tau)$, then $\widehat{A}^\dagger = \widehat{A^*}$.*

Proof. Let $\psi \in \mathcal{H}_\tau$ and $\varphi \in C^\infty_\tau$ such that $\widetilde{\varphi} := \mathbf{1}_B \varphi \in C^\infty_0(\mathbb{R}^d, \mathcal{H})$, where $\mathbf{1}_B$ denotes the characteristic function of the set B. Such φ are dense in $\mathcal{H}_\tau$ and the corresponding $\widetilde{\varphi}$ can be used as a test function:

$$\begin{aligned}
\langle \varphi, \widehat{A}\psi \rangle_{\mathcal{H}_\tau} &= \int_B \mathrm{d}x\, \langle \varphi(x),\, (\widehat{A}\psi)(x) \rangle_{\mathcal{H}} = \int_{\mathbb{R}^d} \mathrm{d}x\, \langle \widetilde{\varphi}(x),\, (\widehat{A}\psi)(x) \rangle_{\mathcal{H}} \\
&= \int_{\mathbb{R}^d} \mathrm{d}x\, \langle (\widehat{A^*}\widetilde{\varphi})(x),\, \psi(x) \rangle_{\mathcal{H}} \\
&= \int_{\mathbb{R}^d} \mathrm{d}x \left\langle \int_{\mathbb{R}^d} \mathrm{d}y\, K_{A^*}(x, y) \widetilde{\varphi}(y),\, \psi(x) \right\rangle_{\mathcal{H}}
\end{aligned}$$

$$
\begin{aligned}
&= \int_{\mathbb{R}^d} \mathrm{d}x \left\langle \int_B \mathrm{d}y\, K_A^*(x,y)\widetilde{\varphi}(y),\, \psi(x) \right\rangle_{\mathcal{H}} \\
&= \int_B \mathrm{d}x \sum_{\gamma\in G} \left\langle \int_B \mathrm{d}y\, K_A^*(x+\gamma,y)\widetilde{\varphi}(y),\, \psi(x+\gamma) \right\rangle_{\mathcal{H}} \\
&= \int_B \mathrm{d}x \sum_{\gamma\in G} \left\langle \int_B \mathrm{d}y\, \tau^{-1}(\gamma) K_A^*(x,y-\gamma)\tau(\gamma)\widetilde{\varphi}(y),\, \tau^{-1}(\gamma)\psi(x) \right\rangle_{\mathcal{H}} \\
&= \int_B \mathrm{d}x \sum_{\gamma\in G} \left\langle \int_B \mathrm{d}y\, K_A^*(x,y-\gamma)\varphi(y-\gamma),\, \psi(x) \right\rangle_{\mathcal{H}} \\
&= \int_B \mathrm{d}x \left\langle \int_{\mathbb{R}^d} \mathrm{d}y\, K_A^*(x,y)\varphi(y),\, \psi(x) \right\rangle_{\mathcal{H}} \\
&= \int_B \mathrm{d}x\, \langle (\widehat{A^*}\varphi)(x),\, \psi(x)\rangle_{\mathcal{H}} = \langle \widehat{A^*}\varphi, \psi\rangle_{\mathcal{H}_\tau}
\end{aligned}
$$

In particular, we used the τ-equivariance of the kernel (5.10) and of the functions in $\mathcal{H}_\tau$ and the unitarity of τ. By density we have $\widehat{A^*} = \widehat{A}^\dagger$. □

Remark 29 (A bundle theoretic rephrasing). The previous construction can be nicely understood in the framework of the theory of G-bundles (see Steenrod, Husemoller, Eilenberg, ...). This rephrasing gives a geometrical understanding of the construction, but it is not needed as far as the applications in Sec. 6.3 are concerned.

The universal covering $\mathbb{R}^d \xrightarrow{\pi} \mathbb{T}^d$ defines a principal G-bundle with structural group $G = \mathbb{Z}^d$, which will be simply denoted as P. To any representation $\tau : \mathbb{Z}^d \to \mathcal{U}(\mathcal{H})$ of the structural group corresponds, in a canonical way, an Hilbert space G-bundle, called the τ-associated bundle and usually denoted as $P \times_\tau \mathcal{H}_\mathrm{f}$. Notice that the previous bundles are trivial as $\mathcal{U}(\mathcal{H})$-bundles whenever $\dim \mathcal{H} = +\infty$ (since $\mathcal{U}(\mathcal{H})$ is contractible in such a case) but they are in general not trivial as $\mathbb{Z}^d$-bundles.

It is well known the following crucial fact: a continuous section of the bundle $P \times_\tau \mathcal{H}$ can be regarded as a τ-equivariant $\mathcal{H}$-valued function on the total space of the principal bundle P, i.e.

$$
C^0(P \times_\tau \mathcal{H}_\mathrm{f}) \cong \left\{ \varphi : \mathbb{R}^d \xrightarrow{C^0} \mathcal{H}_\mathrm{f} : \varphi(x+\gamma) = \tau(\gamma)^{-1}\varphi(x) \right\}
$$

in the category of Banach spaces. In a similar way, locally-H^s sections (defined as sections that are H^s_{loc} with respect to an atlas of local G-trivializations) can be seen as locally-H^s equivariant functions,

$$
L^2(P \times_\tau \mathcal{H}_\mathrm{f}) \cong \left\{ \varphi : \mathbb{R}^d \xrightarrow{L^2_{loc}} \mathcal{H}_\mathrm{f} : \varphi(x+\gamma) = \tau(\gamma)^{-1}\varphi(x) \right\} \equiv \mathcal{H}_\tau
$$

$$H^s(P \times_\tau \mathcal{H}_\mathrm{f}) \cong \left\{ \varphi : \mathbb{R}^d \xrightarrow{H^s} \mathcal{H}_\mathrm{f} : \varphi(x+\gamma) = \tau(\gamma)^{-1}\varphi(x) \right\}.$$

In the same spirit, one notices that τ-equivariant symbols are nothing but morphisms of $P \times_\tau \mathcal{H}$, regarded as an an Hilbert space G-bundles over the torus with fixed base space. $\diamondsuit$

Chapter 6

Effective dynamics for the Bloch electron

6.1 Introduction

An outstanding problem of solid state physics is to understand the motion of electrons in a periodic potential which is generated by the ionic cores. While this problem is quantum mechanical, many electronic properties of solids can be understood already in the semiclassical approximation [AsMe, Ko, Za]. One argues that for suitable wave packets, which spread over many lattice spacings, the main effect of a periodic potential V_Γ on the electron dynamics correspond to changing the dispersion relation from the free kinetic energy $E_{\text{free}}(k) = \frac{1}{2}k^2$ to the modified kinetic energy $E_n(k)$ given by the n^{th} Bloch function. Otherwise the electron responds to external potentials A, W as in the case of vanishing periodic potential. Thus the semiclassical equations of motion

$$\dot{r} = \nabla_k H_{\text{sc}}(r,k)\,, \qquad \dot{k} = -\nabla_r H_{\text{sc}}(r,k) \tag{6.1}$$

are generated by the hamiltonian

$$H_{\text{sc}}(r,k) = E_n(k - A(r)) + W(r)\,, \tag{6.2}$$

where r is the position and k the quasimomentum of the electron. Note that there is a semiclassical evolution for each Bloch band separately.

One of the main goals of this chapter is to understand on a mathematical level how these semiclassical equations emerge from the underlying Schrödinger equation

$$\mathrm{i}\,\partial_t\,\psi(x,t) = \big(\tfrac{1}{2}(-\mathrm{i}\nabla_x + A(\varepsilon x))^2 + V_\Gamma(x) + W(\varepsilon x)\big)\,\psi(x,t) \tag{6.3}$$

in the limit $\varepsilon \to 0$ at leading order and to determine ε-dependent higher order corrections. In (6.3) the potential $V_\Gamma : \mathbb{R}^d \to \mathbb{R}$ is periodic with respect to some regular lattice Γ generated through the basis $\{\gamma_1, \ldots, \gamma_d\}$, $\gamma_j \in \mathbb{R}^d$, i.e.

$$\Gamma = \left\{ x \in \mathbb{R}^d : x = \sum_{j=1}^{d} \alpha_j \gamma_j \text{ for some } \alpha \in \mathbb{Z}^d \right\}$$

and $V_\Gamma(\cdot + \gamma) = V_\Gamma(\cdot)$ for all $\gamma \in \Gamma$. The lattice spacing defines the microscopic spatial scale. The external potentials $A(\varepsilon x)$ and $W(\varepsilon x)$, with $A : \mathbb{R}^d \to \mathbb{R}^d$ and $W : \mathbb{R}^d \to \mathbb{R}$, are slowly varying on the scale of the lattice, as expressed through the dimensionless scale parameter ε, $\varepsilon \ll 1$. In particular, this means that the external fields are weak compared to the fields generated by the ionic cores, a condition which is satisfied for real metals even for the strongest external electrostatic fields available and for a wide range of magnetic fields, cf. [AsMe], Chapter 13.

Note that the external forces due to A and W are of order ε and therefore have to act over a time of order ε^{-1} to produce finite changes, which defines the macroscopic time scale. We will mostly work in the microscopic coordinates (x, t) of (6.3). For sake of comparison we note that the macroscopic space-time scale (x', t') is defined through $x' = \varepsilon x$ and $t' = \varepsilon t$. With this scale change Equation (6.3) reads

$$\mathrm{i}\,\varepsilon\, \partial_{t'}\, \psi^\varepsilon(x', t') = \left(\tfrac{1}{2}(- \mathrm{i}\varepsilon\nabla_{x'} + A(x'))^2 + V_\Gamma(x'/\varepsilon) + W(x')\right) \psi^\varepsilon(x', t') \qquad (6.4)$$

with initial conditions $\psi^\varepsilon(x') = \varepsilon^{-d/2}\psi(x'/\varepsilon)$. If $V_\Gamma = 0$, Equation (6.4) is the usual semiclassical limit with ε set equal to $\hbar$.

The problem of deriving (6.1) from (6.3) in the limit $\varepsilon \to 0$ has been attacked along several routes. In the physics literature (6.1) is usually accounted for by constructing suitable semiclassical wave packets, cf. [Ko, Za]. The few mathematical approaches to the time-dependent problem consider (6.4) and extend techniques from semiclassical analysis as the WKB ansatz [GRT] or Wigner measures [GMMP, MMP] to the modified picture. However, in [GRT] a constant magnetic field and no electric field is assumed, while in [GMMP, MMP] there are no external fields at all.

To get a better understanding note that the step from (6.3) to (6.1) involves actually two limits. Semiclassical behavior can only emerge if a Bloch band is separated by a gap from the other bands and thus the corresponding subspace decouples adiabatically from its orthogonal complement. In [HST], where the semiclassical model (6.1) is derived for the case of zero magnetic field, the adiabatic decoupling and the semiclassical limit are carefully separated. First it is shown that Bloch subspaces corresponding to isolated bands are approximately

invariant under the time evolution. Secondly the effective hamiltonian which generates the dynamics inside such a subspace is determined. As a third step one obtains the semiclassical equations of motion (6.1) as the semiclassical limit of the effective dynamics.

The present Chapter is, in spirit, a continuation of the program started in [HST] to the case of both, external magnetic and electric fields. Our results constitute not only the first derivation of the semiclassical model in this generality, but they add, as we shall explain, new insight to the structure of the problem and allow to compute higher order corrections to the semiclassical equations.

Since the precise statements of our results require considerable technical preparations, they are postponed to Section 6.3. At this point we briefly describe some easy to formulate but central consequences of our main results. For this we write the unitary group which provides the solutions to (6.3) in $\mathcal{H} := L^2(\mathbb{R}^d)$ as $\mathrm{e}^{-\mathrm{i}H^\varepsilon t}$, $t \in \mathbb{R}$, with hamiltonian

$$H^\varepsilon = \tfrac{1}{2}\big(-\mathrm{i}\nabla_x + A(\varepsilon x)\big)^2 + V_\Gamma(x) + W(\varepsilon x)\,. \tag{6.5}$$

We will assume that A and W are smooth and bounded together with all their derivatives.

For each Bloch band $E_n(k)$ which does not cross or touch any other Bloch band we construct an orthogonal projector Π_n^ε such that the associated subspace $\Pi_n^\varepsilon\mathcal{H}$ of the full Hilbert space $\mathcal{H}$ is approximately invariant under the time evolution. More precisely, Π_n^ε satisfies

$$\| [H^\varepsilon, \Pi_n^\varepsilon] \|_{\mathcal{B}(\mathcal{H})} = \mathcal{O}(\varepsilon^\infty)$$

and thus

$$\| [\mathrm{e}^{-\mathrm{i}H^\varepsilon t}, \Pi_n^\varepsilon] \|_{\mathcal{B}(\mathcal{H})} = \mathcal{O}(\varepsilon^\infty |t|)\,.$$

Recall that a function $q : (0, \varepsilon_0) \to [0, \infty)$ is $\mathcal{O}(\varepsilon^\infty)$, if for every $m \in \mathbb{N}$ there is a constant $C_m < \infty$, such that $q(\varepsilon) \leq C_m \varepsilon^m$. Hence transitions between $\Pi_n^\varepsilon\mathcal{H}$ and its orthogonal complement $(\Pi_n^\varepsilon\mathcal{H})^\perp$ are asymptotically smaller than any power of ε *uniformly for all initial states.* In this sense $\Pi_n^\varepsilon\mathcal{H}$ is an adiabatically decoupled subspace.

As the seconds step we show that on this subspace the hamiltonian H^ε allows for an asymptotic expansion in ε with the zeroth order term given through Peierls substitution, i.e.

$$H^\varepsilon\Pi_n^\varepsilon = \Big(E_n\big(-\mathrm{i}\nabla_x + A(\varepsilon x)\big) + W(\varepsilon x)\Big)\,\Pi_n^\varepsilon + \mathcal{O}(\varepsilon)\,,$$

where $\mathcal{O}(\varepsilon)$ holds in the norm of $\mathcal{B}(\mathcal{H})$, the space of bounded operators on $\mathcal{H}$. The operator $E_n\big(-\mathrm{i}\nabla_x + A(\varepsilon x)\big)$ has to be understood in the sense of Weyl quantization.

We remark that the natural representation for the study of the effective hamiltonian is the Bloch-Floquet representation. As we do not want to burden the introduction with technicalities, we only mention that our results allow, in particular, to compute corrections to Peierls substitution, that is higher order terms in the expansion of $\Pi_n^\varepsilon H^\varepsilon \Pi_n^\varepsilon$. We shall explicitly compute and discuss the first order correction.

Since all errors in our results are small in the norm of bounded operators and thus uniformly in all initial states, the third step, i.e. the semiclassical analysis of the effective Schrödinger equation on the decoupled band subspace, is straightforward. We will exemplify this point by proving an Egorov theorem with classical flow Φ_n^t given through the semiclassical model (6.1). To leading order, the semiclassical observables are those functions on phase space $\mathbb{R}^{2d}$, which are Γ^*-periodic in the second argument, where Γ^* is the dual lattice.

Corollary 30. *Let $A \in C_{\mathrm{b}}^\infty(\mathbb{R}^{2d})$ be Γ^*-periodic, i.e. $A(r, k+\gamma^*) = A(r,k)$ for all $\gamma^* \in \Gamma^*$, and let $\widehat{A} = A(\varepsilon x, -\mathrm{i}\nabla_x)$ be understood in the sense of Weyl quantization. Then the corresponding time-evolved Heisenberg observable is approximately given through the quantization of the classically transported function,*

$$\left\| \left(\mathrm{e}^{\mathrm{i}H^\varepsilon t/\varepsilon}\, \widehat{A}\, \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} \;-\; \widehat{A}(\Phi_n^{-t}(r,k)) \right) \Pi_n^\varepsilon \right\| = \mathcal{O}(\varepsilon)\,. \tag{6.6}$$

Note that the results presented in Section 2 contain much stronger and more detailed statements than Corollary 30, but require several technical prerequisites for their formulation, which we decided to omit in the introduction. Still Corollary 30 is, to our knowledge, the first rigorous result relating the full time-dependent Schrödinger equation (6.3) to the semiclassical model (6.1) for general external magnetic and electric fields.

Let us give a brief plan of the Chapter. In Section 2 we present and discuss our main results in full detail after introducing the necessary concepts and assumptions. The proofs are given in Section 3 and are an adaption of a general perturbative scheme as developed in [PST$_1$], see also [NeSo], to the present setting. As mentioned and as to be explained in more detail, the problem at hand is first an adiabatic problem and only on the adiabatically decoupled subspaces a semiclassical one. The key observation for applying space-adiabatic perturbation theory as in [PST$_1$] is that the hamiltonian H^ε can be written, after a suitable Bloch-Floquet transformation, as the Weyl quantization of an operator valued symbol. However, the underlying Hilbert space is not of the form $L^2(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}})$, as for usual Weyl quantization, but $L^2(B, \mathcal{H}_{\mathrm{f}})$, where B is the first Brillouin zone, the fundamental domain of the dual lattice Γ^*. And the symbols are not functions on the phase space $\mathbb{R}^d \times \mathbb{R}^d$, but on $B \times \mathbb{R}^d$. Hence a suitable version of the parameter dependent pseudodifferential calculus needs to be developed in Section 4.

6.2 Dynamics in periodic structures: setup and main results

6.2.1 The Bloch-Floquet transform

The dual lattice Γ^* is defined as the lattice generated by the dual basis $\{\gamma_1^*, \ldots, \gamma_d^*\}$ determined through the conditions $\gamma_i \cdot \gamma_j^* = 2\pi\delta_{ij}$, $i, j \in \{1, \ldots, d\}$. The centered fundamental domain of Γ is denoted by

$$M = \left\{ x \in \mathbb{R}^d : x = \sum_{j=1}^{d} \alpha_j \gamma_j \text{ for } \alpha_j \in [-\tfrac{1}{2}, \tfrac{1}{2}] \right\}, \tag{6.7}$$

and analogously the centered fundamental domain of Γ^* is denoted by M^*. In solid state physics the set M^* is called the *first Brillouin zone*, and for this reason we will denote it as B. In the following M^* is always equipped with *normalized* Lebesgue measure denoted by $\mathrm{d}k$. We introduce the notation $x = [x] + \gamma$ for the a.e. unique decomposition of $x \in \mathbb{R}^d$ as a sum of $[x] \in M$ and $\gamma \in \Gamma$. We use the same brackets for the analogous splitting $k = [k] + \gamma^*$.

It is convenient to define the Bloch-Floquet transformation as

$$(\mathcal{U}\psi)(k, x) := \sum_{\gamma \in \Gamma} \mathrm{e}^{-i(x+\gamma)\cdot k} \psi(x + \gamma), \quad (k, x) \in \mathbb{R}^{2d}, \tag{6.8}$$

for any $\psi \in \mathcal{S}(\mathbb{R}^d)$. Clearly, one finds the following periodicity properties:

$$(\mathcal{U}\psi)(k, y + \gamma) = (\mathcal{U}\psi)(k, y) \quad \text{for all} \quad \gamma \in \Gamma \tag{6.9}$$

$$(\mathcal{U}\psi)(k + \gamma^*, y) = \mathrm{e}^{-\mathrm{i}y\cdot\gamma^*} (\mathcal{U}\psi)(k, y) \quad \text{for all} \quad \gamma^* \in \Gamma^*. \tag{6.10}$$

From (6.9) it follows that, for any fixed $k \in \mathbb{R}^d$, $(\mathcal{U}\psi)(k, \cdot)$, is a Γ-periodic function and can then be regarded as an element of $L^2(\mathbb{T}^d)$, $\mathbb{T}^d$ being the flat torus, i.e. $\mathbb{T}^d := \mathbb{R}^d/\Gamma$. Notice that the distinction between the naturally isomorphic spaces $L^2(\mathbb{T}^d)$ and $L^2(M)$ is meaningful, and useful to avoid confusion, when one focuses on a subspace of continuous functions.

Moreover, one notices that (6.10) involves a unitary representation of the group of lattice translation on Γ^* (denoted again as Γ^* with a little abuse of notation), given by

$$\tau : \Gamma^* \to \mathcal{U}(L^2(\mathbb{T}^d)), \quad \gamma^* \mapsto \tau(\gamma^*) \tag{6.11}$$

where $\tau(\gamma^*)$ is given by multiplication times $\mathrm{e}^{\mathrm{i}y\cdot\gamma^*}$ in $L^2(\mathbb{T}^d, dy)$. It is then convenient to introduce the Hilbert space

$$\mathcal{H}_\tau := \left\{ \psi \in L^2_{\mathrm{loc}}(\mathbb{R}^d, L^2(\mathbb{T}^d)) : \ \psi(k - \gamma^*) = \tau(\gamma^*)\, \psi(k) \right\}, \tag{6.12}$$

equipped with the inner product

$$\langle \psi,\, \varphi \rangle_{\mathcal{H}_\tau} = \int_B \mathrm{d}k\, \langle \psi(k),\, \varphi(k) \rangle_{L^2(\mathbb{T})}\,.$$

Notice that if one considers the trivial representation, i.e. $\tau \equiv 1$, then $\mathcal{H}_\tau$ is nothing but a space of Γ^*-periodic vector-valued functions over $\mathbb{R}^d$.

Obviously, there is a natural isomorphism between $\mathcal{H}_\tau$ and $L^2(B, L^2(\mathbb{T}^d))$ given by restriction from $\mathbb{R}^d$ to B, and with inverse given by τ-equivariant continuation, as suggested by (6.10). The reason for working with $\mathcal{H}_\tau$ instead of $L^2(B, L^2(\mathbb{T}^d))$ is twofold. First of all it allows to apply the pseudodifferential calculus as developed in Chapter 5. On the other hand it makes statements about domains of operators more transparent as we shall see.

The map defined by (6.8) extends to a unitary operator

$$\mathcal{U} : L^2(\mathbb{R}^d) \to \mathcal{H}_\tau \cong L^2(B, L^2(\mathbb{T}^d)) \cong L^2(B) \otimes L^2(\mathbb{T}^d) \tag{6.13}$$

The facts that $\mathcal{U}$ is an isometry and that $\mathcal{U}^{-1}$ given through

$$(\mathcal{U}^{-1}\varphi)(x) = \int_B \mathrm{d}k\; \mathrm{e}^{\mathrm{i}x\cdot k}\, \varphi(k, [x]) \tag{6.14}$$

satisfies $\mathcal{U}^{-1}\mathcal{U}\psi = \psi$ for $\psi \in \mathcal{S}(\mathbb{R}^d)$ can be checked by direct calculation. It is also straightforward to check that $\mathcal{U}^{-1}$ extends to an isometry from $\mathcal{H}_\tau$ to $L^2(\mathbb{R}^d)$. Hence $\mathcal{U}^{-1}$ must be injective and as a consequence U must be surjective and thus unitary.

Next we discuss how differential and multiplication operators behave under Bloch-Floquet transformation. The following assertions follow in a straightforward way from the definition (6.8). Let $P = -\mathrm{i}\nabla_x$ with domain $H^1(\mathbb{R}^d)$ and Q be multiplication with x on the maximal domain, then

$$\mathcal{U}\, P\, \mathcal{U}^{-1} \;=\; 1 \otimes -\mathrm{i}\nabla_y^{per} + k \otimes 1 \tag{6.15}$$

$$\mathcal{U}\, Q\, \mathcal{U}^{-1} \;=\; \mathrm{i}\nabla_k^{\tau}\,, \tag{6.16}$$

where $-\mathrm{i}\nabla_y^{per}$ is equipped with periodic boundary conditions or, equivalently, operating on the domain $H^1(\mathbb{T}^d)$. The domain of $\mathrm{i}\nabla_k^\tau$ is $\mathcal{H}_\tau \cap H^1_{\mathrm{loc}}(\mathbb{R}^d, L^2(\mathbb{T}))$, i.e. it consists of distributions in $H^1(B, L^2(\mathbb{T}^d))$ which satisfy the y-dependent boundary condition associated with (6.10).

The central feature of the Bloch-Floquet transformation is, however, that multiplication with a Γ periodic function like V_Γ is mapped into multiplication with the same function, i.e. $\mathcal{U}\, V_\Gamma(x)\, \mathcal{U}^{-1} = \mathbf{1} \otimes V_\Gamma(y)$.

6.2.2 The free hamiltonian

Equipped with this remarks, one notice that the Bloch-Floquet transform of the free hamiltonian

$$H_{\rm per} := -\frac{1}{2}\Delta + V_\Gamma \tag{6.17}$$

is given by

$$\mathcal{U}\, H_{\rm per}\, \mathcal{U}^{-1} = \int_B^\oplus \mathrm{d}k\, H_{\rm per}(k) \tag{6.18}$$

with

$$H_{\rm per}(k) = \frac{1}{2}(-\mathrm{i}\nabla_y + k)^2 + V_\Gamma(y)\,, \quad k \in B\,. \tag{6.19}$$

$H_{\rm per}(k)$ acts on $L^2(\mathbb{T}^d)$ with domain $H^2(\mathbb{T}^d)$ independent of $k \in B$.

Remark 31. *The reason for taking the particular form of the Bloch-Floquet transform given in(6.8) is that the domain of $H_{\rm per}(k)$ is independent of k that way.* $\diamondsuit$

Before going on with the analysis of (6.19) we state the assumptions on the potentials.

Assumption (A_1). We assume that V_Γ is infinitesimally bounded with respect to $-\Delta$ and that $W \in C^\infty_{\rm b}(\mathbb{R}^d, \mathbb{R})$ and $A_i \in C^\infty_{\rm b}(\mathbb{R}^d, \mathbb{R})$ for any $i \in \{1, \ldots, d\}$. $\diamondsuit$

From this assumption it follows in particular that H^ε is self-adjoint on $H^2(\mathbb{R}^d)$. The previous assumption excludes the case of globally constant electric and magnetic field. However, for the questions we shall address, locally constant fields can be considered in place of globally constant fields.

The resolvent $R^0_\lambda = (H_0(k) - \lambda)^{-1}$ of the operator $H_0(k) = \frac{1}{2}(-\mathrm{i}\nabla_y + k)^2$ is compact for fixed $k \in B$. Since, by assumption, $R_\lambda V_\Gamma$ is bounded, also $R_\lambda = (H_{\rm per}(k) - \lambda)^{-1} = R^0_\lambda + R_\lambda V_\Gamma R^0_\lambda$ is compact. As a consequence $H_{\rm per}(k)$ has purely discrete spectrum with eigenvalues of finite multiplicity which accumulate at infinity. For definiteness the eigenvalues are enumerated according to their magnitude, $E_1(k) \leq E_2(k) \leq E_3(k) \leq \ldots$ and repeated according to their multiplicity. The corresponding normalized eigenfunctions $\{\varphi_n(k)\}_{n\in\mathbb{N}} \subset H^2(\mathbb{T}^d)$ are called Bloch functions and form, for any fixed k, an orthonormal basis of $L^2(\mathbb{T}^d)$. We will call $E_n(k)$ the $n^{\rm th}$ band function. Notice that, with this choice of the labelling, $E_n(k)$ and $\varphi_n(k)$ are generally *not* smooth functions of k if eigenvalue crossings are present. Since

$$H_{\rm per}(k - \gamma^*) = \tau(\gamma^*)\, H_{\rm per}(k)\, \tau(\gamma^*)^{-1}\,, \tag{6.20}$$

the band functions $E_n(k)$ are periodic with respect to Γ^*.

Definition 32. *We say that a band $E_n(k)$ or a group of bands $\{E_n(k)\}_{n\in\mathcal{I}}$, $\mathcal{I} = [I_-, I_+] \cap \mathbb{N}$, is an* ***isolated energy band****, if*

$$\inf_{k\in B} \operatorname{dist}\Big(\bigcup_{n\in\mathcal{I}} \{E_n(k)\},\ \bigcup_{m\notin\mathcal{I}} \{E_m(k)\} \Big) =: C_{\mathrm{g}} > 0\,. \tag{6.21}$$

$\diamondsuit$

For the following we fix an index set $\mathcal{I} \subset \mathbb{N}$ corresponding to an isolated group of bands. Clearly from Def. 32 it follows that there exists an interval $\mathcal{J}(k) := [J_-(k), J_+(k)]$, defined by smooth and periodic functions $J_\pm : \mathbb{R}^d \to \mathbb{R}$, such that:

(i) $\bigcup_{n\in\mathcal{I}}\{E_n(k)\} \subset \mathcal{J}(k)$ for any $k \in B$

(ii) $\inf_{k\in B} \operatorname{dist}\Big(\mathcal{J}(k),\ \bigcup_{m\notin\mathcal{I}}\{E_m(k)\} \Big) \geq \frac{3}{4}\, C_{\mathrm{g}}$

Let $P_{\mathcal{I}}(k)$ be the spectral projector of $H_{\mathrm{per}}(k)$ relative to the interval $\mathcal{J}(k)$. Clearly, $P_{\mathcal{I}}(k)$ does not depend on the choice of $\mathcal{J}(k)$ but only on the set $\mathcal{I} \subset \mathbb{N}$. Then $P_{\mathcal{I}} := \int_B^{\oplus} \mathrm{d}k\, P_{\mathcal{I}}(k)$ is, by definition, the projector on the given isolated energy band.

In terms of Bloch functions, one has that $P_{\mathcal{I}}(k) = \sum_{n\in\mathcal{I}} |\varphi_n(k)\rangle\langle\varphi_n(k)|$. However, in general $\varphi_n(k)$ are not smooth functions of k if eigenvalue crossing are present, while $P_{\mathcal{I}}(k)$ is, by construction, a smooth function of k. Moreover, from (6.20) it follows that

$$P_{\mathcal{I}}(k - \gamma^*) = \tau(\gamma^*)\, P_{\mathcal{I}}(k)\, \tau(\gamma^*)^{-1}. \tag{6.22}$$

We will need the following assumption. For the meaning of τ-equivariance see Def. 21.

Assumption (A_2) Given an isolated group of bands $\{E_n(k)\}_{n\in\mathcal{I}}$, we assume that there exists an orthonormal basis $\{\psi_i(k)\}_{i=1}^m$ of $\mathrm{Ran}P_{\mathcal{I}}(k)$ whose elements are smooth and τ-equivariant with respect to k. $\diamondsuit$

The meaning of this assumption, and the condition under which is satisfied will be discussed in Section 6.3. For the moment, we just notice the following. In the special but important case in which the relevant band consist of an isolated m-fold degenerate eigenvalue (i.e. $E_n(k) = E_*(k)$ for every $n \in \mathcal{I}$, $|\mathcal{I}| = m$) Assumption (A_2) is equivalent to the existence of an orthonormal basis consisting of smooth and τ-periodic Bloch functions. However, in the general case, in which *eigenvalue crossings* inside the relevant band are eventually present, Assumption (A_2) is weaker, since each $\psi_i(k)$ is not required to be eigenfunctions of the free hamiltonian $H_{\mathrm{per}}(k)$ but only of the corresponding eigenprojector $P_{\mathcal{I}}(k)$.

Let $P_n(k) = |\varphi_n(k)\rangle\langle\varphi_n(k)|$, then the projector on the n^{th} band subspace is given through $P_n = \int_B^{\oplus} \mathrm{d}k\, P_n(k)$ and $P_{\mathcal{I}} = \sum_{n\in\mathcal{I}} P_n$. By construction the band subspaces are invariant under the dynamics generated by H_{per},

$$\left[\mathrm{e}^{-\mathrm{i}\mathcal{U}H_{\text{per}}\mathcal{U}^{-1}s},\, P_n\right] = \left[\mathrm{e}^{-\mathrm{i}E_n(k)s},\, P_n\right] = 0 \quad \text{for all } n\in\mathbb{N},\ s\in\mathbb{R}.$$

In the original representation H_{per} acts on the n^{th} band subspace as

$$H_{\text{per}}\psi = \mathcal{U}^{-1}(E_n(k)\otimes\mathbf{1})\mathcal{U}\,\psi = E_n(-\mathrm{i}\nabla_x)\,\psi\,,$$

where $\psi \in \mathcal{U}^{-1}P_n\mathcal{U}\,L^2(\mathbb{R}^d)$. In other words, wave functions in the n^{th} band subspace propagate freely but with a modified dispersion relation given through the n^{th} band function.

The main question we shall address in this Chapter is weather this picture still holds approximately true in the case in which slowly-varying external electromagnetic potential are present. In particular: there exist a correspondence between isolated energy bands and subspaces which are almost-invariant under the time evolution, as $\mathrm{Ran}P_n$ is invariant under the free evolution? Is it possible to describe the dynamics in one of these subspace by an appropriate *effective hamiltonian*, as $E_n(-\mathrm{i}\nabla_x)$ describes the dynamics in the free case? How can this effective hamiltonian be computed? How the error implicit in this approximation can be controlled?

6.2.3 The main result

In this subsection we shall answer the previous questions, referring to Section 6.3 for more detailed results and rigorous proofs.

Generalizing from (6.12) it is convenient to introduce the following notation. For any separable Hilbert space $\mathcal{H}_{\text{f}}$ and any unitary representation $\tau : \Gamma^* \to \mathcal{U}(\mathcal{H}_{\text{f}})$, one defines the Hilbert space

$$L^2_\tau(\mathbb{R}^d, \mathcal{H}_{\text{f}}) := \left\{\psi \in L^2_{\text{loc}}(\mathbb{R}^d, \mathcal{H}_{\text{f}}) :\ \psi(k-\gamma^*) = \tau(\gamma^*)\,\psi(k)\right\}, \tag{6.23}$$

equipped with the inner product

$$\langle\psi,\,\varphi\rangle_{L^2_\tau} = \int_B \mathrm{d}k\,\langle\psi(k),\,\varphi(k)\rangle_{\mathcal{H}_{\text{f}}}\,.$$

Using the results of the previous section and imposing Assumption (A1), the Bloch-Floquet transform of the full hamiltonian (6.5) is given through

$$H^\varepsilon_{\text{BF}} := \mathcal{U}\,H^\varepsilon\,\mathcal{U}^{-1} = \frac{1}{2}\Big(-\mathrm{i}\nabla_y + k - A(\mathrm{i}\varepsilon\nabla^\tau_k)\Big)^2 + V_\Gamma(y) + W(\mathrm{i}\varepsilon\nabla^\tau_k) \tag{6.24}$$

with domain $L^2_\tau(\mathbb{R}^d, H^2(\mathbb{T}^d))$.

As previously pointed out, one expects that, for any initial datum in a suitable almost-invariant subspace, the true dynamics is close to an effective dynamics. In particular, if one considers an isolated group of bands $\{E_n(k)\}_{n\in\mathcal{I}}$ the effective dynamics is described in the Hilbert space $\mathcal{K}_{\rm ref} \cong L^2(\mathbb{T}^d)\otimes\mathbb{C}^m$ with $m := \dim P_{\mathcal{I}}(k)$.

Theorem 33 (Peierl's substitution and higher order corrections). *Let $\{E_n\}_{n\in\mathcal{I}}$ be an isolated group of bands, see Definition 32, and let Assumptions (A_1) and (A_2) be satisfied. Then there exists an orthogonal projection $\Pi^\varepsilon \in \mathcal{B}(\mathcal{H}_\tau)$ such that*

$$[\, H^\varepsilon_{\rm BF},\, \Pi^\varepsilon\,] = \mathcal{O}_0(\varepsilon^\infty) \tag{6.25}$$

and there exist a partial isometry $U \in \mathcal{B}(\mathcal{H}_\tau, \mathcal{K}_{\rm ref})$ and an hermitian operator $\widehat{h}_{\rm eff} \in \mathcal{B}(\mathcal{K}_{\rm ref})$ so that

$$(e^{-iH^\varepsilon_{\rm BF}t} - U\; e^{-i\widehat{h}_{\rm eff}t}\; U^*)\Pi^\varepsilon = \mathcal{O}_0(\varepsilon^\infty|t|). \tag{6.26}$$

Moreover $\widehat{h}_{\rm eff}$ is the Weyl quantization (in the sense of Section 5) of a semiclassical symbol $h_{\rm eff} \in M^\varepsilon_{\tau\equiv 1}(1, \mathcal{B}(\mathbb{C}^m))$ which allow for an asymptotic expansion in ε which can be computed at any order.

In particular, for an isolated m-fold degenerate eigenvalue $E_{\rm r}(k)$ the $\mathcal{B}(\mathbb{C}^m)$-valued symbol $h_{\rm eff}(k,r) = h_0(k,r) + \varepsilon h_1(k,r) + \mathcal{O}_0(\varepsilon^2)$ has matrix-elements

$$h_0(k,r)_{\alpha\beta} = (E(k - A(r)) + W(r))\delta_{\alpha\beta} \tag{6.27}$$

and, for $d = 3$,

$$\begin{aligned} h_1(k,r)_{\alpha\beta} &= (\nabla W(r) - (v(\tilde{k}) \wedge B(r))) \cdot A_{\rm Berry}(\tilde{k})_{\alpha\beta} \\ &- \frac{i}{2}\, B(r) \cdot \langle \nabla\psi_\alpha(\tilde{k}),\; \wedge(H_{\rm per}(\tilde{k}) - E(\tilde{k}))\nabla\psi_\beta(\tilde{k})\rangle_{\mathcal{H}_{\rm f}} \end{aligned} \tag{6.28}$$

where $\alpha, \beta \in \{1, \ldots, m\}$ and we abbreviated $B = {\rm d}A$, $\tilde{k} = k - A(r)$, $v(k) = \nabla E(k)$ and

$$A_{\rm Berry}(k)_{\alpha\beta} = i\langle\psi_\alpha(k), \nabla\psi_\beta(k)\rangle. \tag{6.29}$$

The physical interpretation of the effective hamiltonian $\widehat{h}_{\rm eff}$ is the following. The zero-order term (6.27) corresponds to the well-known **Peierl's substitution** (references) and express the fact that an electron in a periodic potential propagates, at the leading order, as a free electron with modified dispersion relation given by $E_{\rm r}(k)$. Moreover, the fact that the physical velocity is given by $\tilde{v}(k,r) := \nabla E_{\rm r}(k - A(r)) = v(\tilde{k})$ suggests that, for $m = 1$, the first order term

$$h_1(k,r) = -A_{\rm Berry}(\tilde{k}) \cdot F_{\rm Lor}(r, \tilde{v}(k,r)) - M(\tilde{k}) \cdot B(r)$$

can be regarded as the sum of the energy of an electric dipole with velocity dependent momentum $A_{\text{Berry}}(\tilde{k})$ and the energy of a magnetic dipole with velocity dependent momentum $M(\tilde{k})$. As suggested by the notation, $A_{\text{Berry}}(\tilde{k})$ corresponds to a (generalized) Berry connection, i.e. a $U(m)$-connection on a suitable $U(m)$-bundle.

Theorem 33 is a direct consequence of the results proved in Prop. 34, 36, 37 and 38.

6.3 Mathematical proofs

In this section we proof a number of propositions that, in particular, imply our main result, namely Theorem 33. The main idea of the proof is to adapt to the case of the Bloch electron the general scheme of space-adiabatic perturbation theory, developed in [PST$_1$] and related to previous works by Blount [Bl$_1$], Littlejohn and coworkers ([LiFl],[LiWe]) and Nenciu and Sordoni [NeSo].

To this end, one has to face two mathematical problems. First of all, one has to face the fact that in the present case the symbols are *unbounded*-operator-valued functions. The second problem consists in generalizing the Weyl calculus to operator-valued functions defined over the cotangent bundle of the torus or, more generally, to morphism of (non trivial) Hilbert-space bundles over the torus. This goal is achieved by the theory developed in Ch. 5. In this section, we will widely use terminology and notations introduced there.

Equipped with the concepts and the terminology introduced in the Appendix, we notice that the hamiltonian $H^{\varepsilon}_{\text{BF}}$ is the Weyl quantization of the τ-equivariant symbol

$$H_0(k,r) = \frac{1}{2}\left(-i\nabla_x + k - A(r)\right)^2 + V_{\Gamma}(x) + W(r) \tag{6.30}$$

acting on the Hilbert space $\mathcal{H}_{\text{f}} := L^2(\mathbb{T}^d_x, dx)$ with constant domain $\mathcal{D} := H^2(\mathbb{T}^d)$. For sake of the clarity, we spend two more words on this point. For any fixed $k, r \in \mathbb{R}^d$, $H_0(k,r)$ is regarded as a bounded operator from $\mathcal{D}$ to $\mathcal{H}_{\text{f}}$ which is τ-equivariant with respect to the *bounded* representation $\tau_1 := \tau|_{\mathcal{D}}$ acting on $\mathcal{D}$ and the unitary representation $\tau_2 := \tau$ acting on $\mathcal{H}_{\text{f}}$ (see Def. 22). Then the general theory developed in Sec. 4 can be applied. The (usual) Weyl quantization of H_0 is an operator from $\mathcal{S}'(\mathbb{R}^d, \mathcal{D})$ to $\mathcal{S}'(\mathbb{R}^d, \mathcal{H}_{\text{f}})$ given by

$$\widehat{H}_0 = \frac{1}{2}\Big(-\mathrm{i}\nabla_y + k - A(\mathrm{i}\varepsilon\nabla_k)\Big)^2 + V_{\Gamma}(y) + W(\mathrm{i}\varepsilon\nabla_k) \tag{6.31}$$

where ∇_k is the usual gradient, with domain $H^1(\mathbb{R}^d, \mathcal{D})$. $\widehat{H}_0$ can be restricted to $L^2_{\text{loc}}(\mathbb{R}^d, \mathcal{D})$, since A and W are smooth and bounded. Since H_0 is a τ-equivariant

symbol, then $\widehat{H}_0$ preserves τ-equivariance and can then be restricted to an operator from $L^2_\tau(\mathbb{R}^d, \mathcal{D})$ to $L^2_\tau(\mathbb{R}^d, \mathcal{H}_\mathrm{f})$. To conclude that (6.31), restricted to $L^2_\tau(\mathbb{R}^d, \mathcal{D})$, agrees with (6.24), it is enough to recall that $i\nabla^\tau_k$ is defined as $i\nabla_k$ restricted to $H^1 \cap \mathcal{H}_\tau$ and to use the spectral calculus.

Moreover, if one introduces the order function $w(k, r) := (1 + k^2)$ (see Def. 15), then $H_0 \in S(w, \mathcal{B}(\mathcal{D}, \mathcal{H}))$. More generally, we will give the proofs for any symbol $H \in S^\epsilon(w, \mathcal{B}(\mathcal{D}, \mathcal{H}))$.

6.3.1 The almost invariant subspace

The first result in a space-adiabatic theory is the existence of the almost invariant subspace associated to an isolated group of bands. More introduction....

Given an isolated group of bands $\{E_n(k)\}_{n\in\mathcal{I}}$ we define $\pi_0(k, r)$ as the spectral projector of $H_0(k, r)$ corresponding to the interval $\mathcal{J}(k - A(r))$ introduced after Def. 32. Equivalently, $\pi_0(k, r) := P_\mathcal{I}(k - A(r))$. From both definitions it is clear that $\pi_0 \in S_\tau(1, \mathcal{B}(\mathcal{H}_\mathrm{f}))$. In terms of Bloch functions one has

$$\pi_0(k, r) = \sum_{n\in\mathcal{I}} |\varphi_n(k - A(r))\rangle \langle\varphi_n(k - A(r))| \tag{6.32}$$

However, if eigenvalue crossing inside the relevant band are present the explicit representation (6.32) is not very convenient, since $\varphi_n(k)$ is, in general, either not smooth at the crossing points or not τ-equivariant.

Proposition 34 (Existence of almost invariant subspaces). *Let $\{E_n\}_{n\in\mathcal{I}}$ be an isolated group of bands, see Definition 32, and let Assumption (A_1) be satisfied. Then there exists an orthogonal projection $\Pi^\epsilon \in \mathcal{B}(\mathcal{H}_\tau)$ such that*

$$[\, H^\epsilon_\mathrm{BF},\, \Pi^\epsilon \,] = \mathcal{O}_0(\epsilon^\infty) \tag{6.33}$$

and $\Pi^\epsilon = \widehat{\pi} + \mathcal{O}(\epsilon^\infty)$, where $\widehat{\pi}$ is the Weyl quantization of a τ-equivariant semi-classical symbol

$$\pi \asymp \sum_{j\geq 0} \epsilon^j \pi_j \text{ in } S^\epsilon_\tau(1, \mathcal{B}(\mathcal{H}_\mathrm{f}))$$

whose principal part $\pi_0(k, r)$ is the spectral projector of $H_0(k, r)$ corresponding to the given isolated group of bands.

Proof. The following construction is analogous to the one given in [PST$_1$] with two main differences. The symbol H takes values in the unbounded operators on $\mathcal{H}_\mathrm{f}$ and all symbols appearing are τ-equivariant. Since the necessary changes are not all obvious, we present again the full argument. As in [PST$_1$], the first part

of the proof consist in the construction of a Moyal projector, i.e. a projector at the level of formal symbols.

Lemma 35. *Let* $w(k,r) = (1+k^2)$. *There exists a* unique *formal symbol*

$$\pi = \sum_{j=0}^{\infty} \varepsilon^j \pi_j \quad \in M^{\varepsilon}_{\tau}(1, \mathcal{B}(\mathcal{H}_{\mathrm{f}})) \cap M^{\varepsilon}_{\tau}(w, \mathcal{B}(\mathcal{H}_{\mathrm{f}}, \mathcal{D}))$$

such that $\pi_0(k,r) = P_{\mathcal{I}}(k - A(r))$ *and*

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

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

(iii) $H \# \pi - \pi \# H = 0$.

Proof. As in [PST$_1$] we construct the formal symbol π locally in phase space and obtain by uniqueness, which can be proved as in [PST$_1$], a globally defined formal symbol.

Fix a point $z_0 = (k_0, r_0) \in \mathbb{R}^{2d}$. From the continuity of the map $z \mapsto H(z)$ and the gap condition it follows that there exists a neighborhood $\mathcal{U}_{z_0}$ of z_0 such that for every $z \in \mathcal{U}_{z_0}$ the set $\{E_n(z)\}_{n\in\mathcal{I}}$ can be enclosed by a positively-oriented circle $\Lambda(z_0) \subset \mathbb{C}$ independent of z in such a way that $\Lambda(z_0)$ is symmetric with respect to the real axis,

$$\mathrm{dist}(\Lambda(z_0), \sigma(H(z))) \geq \frac{1}{4} C_{\mathrm{g}} \quad \text{for all} \quad z \in \mathcal{U}_{z_0} \tag{6.34}$$

and

$$\mathrm{Radius}(\Lambda(z_0)) \leq C_{\mathrm{r}}\,. \tag{6.35}$$

The constant C_{g} appearing in (6.34) is the same as in Definition 32 and the existence of a constant C_{r} independent of z_0 such that (6.35) is satisfied follows from the periodicity of $\{E_n(z)\}_{n\in\mathcal{I}}$ and the fact that A and W are bounded. Indeed, Λ can be chosen Γ^*-periodic, i.e. such that $\Lambda(k_0 + \gamma^*, r_0) = \Lambda(k_0, r_0)$ for all $\gamma^* \in \Gamma^*$.

Let us choose any $\zeta \in \Lambda(z_0)$ and restrict all the following expressions to $z \in \mathcal{U}_{z_0}$. We will construct a formal symbol $R(\zeta)$ with values in $\mathcal{B}(\mathcal{H}_{\mathrm{f}}, \mathcal{D})$ – the local Moyal resolvent of H – such that

$$(H - \zeta) \# R(\zeta) = \mathbf{1}_{\mathcal{H}_{\mathrm{f}}} \quad \text{and} \quad R(\zeta) \# (H - \zeta) = \mathbf{1}_{\mathcal{D}} \quad \text{on } \mathcal{U}_{z_0}\,. \tag{6.36}$$

To this end let

$$R_0(\zeta) = (H - \zeta)^{-1}\,,$$

where according to (6.34) $R_0(\zeta)(z) \in \mathcal{B}(\mathcal{H}_\mathrm{f}, \mathcal{D})$ for all $z \in \mathcal{U}_{z_0}$, and, using differentiability of $H(z)$, $\partial_z^\alpha R_0(\zeta)(z) \in \mathcal{B}(\mathcal{H}_\mathrm{f}, \mathcal{D})$ for all $z \in \mathcal{U}_{z_0}$. By construction one has

$$(H - \zeta) \# R_0(\zeta) = \mathbf{1}_{\mathcal{H}_\mathrm{f}} + \mathcal{O}_0(\varepsilon)$$

where the remainder is $\mathcal{O}(\varepsilon)$ in the $\mathcal{B}(\mathcal{H}_\mathrm{f})$-norm. We proceed by induction. Suppose that

$$R^{(n)}(\zeta) = \sum_{j=0}^{n} \varepsilon^j R_j(\zeta)$$

with $R_j(\zeta)(z) \in \mathcal{B}(\mathcal{H}_\mathrm{f}, \mathcal{D})$ for all $z \in \mathcal{U}_{z_0}$ satisfies the first equality in (6.36) up to $\mathcal{O}(\varepsilon^{n+1})$, i.e.

$$(H - \zeta) \# R^{(n)}(\zeta) = \mathbf{1}_{\mathcal{H}_\mathrm{f}} + \varepsilon^{n+1} E_{n+1}(\zeta) + \mathcal{O}_0(\varepsilon^{n+2}), \tag{6.37}$$

where $E_{n+1}(\zeta)(z) \in \mathcal{B}(\mathcal{H}_\mathrm{f})$. By choosing

$$R_{n+1}(\zeta) = -R_0(\zeta)\, E_{n+1} \tag{6.38}$$

we obtain that $R^{(n+1)}(\zeta) = R^{(n)}(\zeta) + \varepsilon^{n+1} R_{n+1}(\zeta)$ takes values in $\mathcal{B}(\mathcal{H}_\mathrm{f}, \mathcal{D})$ and satisfies the first equality in(6.36) up to $\mathcal{O}(\varepsilon^{n+2})$. Hence the formal symbol $R(\zeta) = \sum_{j=0}^{\infty} \varepsilon^j R_j(\zeta)$ constructed that way satisfies the first equality in (6.36) exactly. By the same argument one shows that there exists a formal symbol $\tilde{R}(\zeta)$ with values in $\mathcal{B}(\mathcal{H}_\mathrm{f}, \mathcal{D})$ which exactly satisfies the second equality in (6.36). By the associativity of the Moyal product, they must agree:

$$\tilde{R}(\zeta) = \tilde{R}(\zeta) \# (H - \zeta) \# R(\zeta) = R(\zeta) \qquad \text{on } \mathcal{U}_{z_0}. \tag{6.39}$$

Equations (6.36) imply that $R(\zeta)$ satisfies the resolvent equation

$$R(\zeta) - R(\zeta') = (\zeta - \zeta')\, R(\zeta) \# R(\zeta') \quad \text{on } \mathcal{U}_{z_0} \tag{6.40}$$

for any $\zeta, \zeta' \in \Lambda(z_0)$. From the resolvent equation it follows as in [PST$_1$] that the $\mathcal{B}(\mathcal{H}_\mathrm{f}, \mathcal{D})$-valued formal symbol $\pi = \sum_{j=0}^{\infty} \varepsilon^j \pi_j$ defined through

$$\pi_j(z) := \frac{\mathrm{i}}{2\pi} \oint_{\Lambda(z_0)} \mathrm{d}\zeta\, R_j(\zeta, z) \quad \text{on } \mathcal{U}_{z_0} \tag{6.41}$$

satisfies (i) and (ii) of Lemma 35. As for (iii) a little bit of care is required. Let $J : \mathcal{D} \to \mathcal{H}_\mathrm{f}$ the continuous injection of $\mathcal{D}$ into $\mathcal{H}_\mathrm{f}$. Using (6.41) and (6.40) it follows that $\pi\, J \# R(\zeta) = R(\zeta)\, J \# \pi$ for all $\zeta \in \Lambda(z_0)$. Moyal-multiplying from left and from the right with $H - \zeta$ one finds $H \# \pi\, J = J\, \pi \# H$ as operators in

$\mathcal{B}(\mathcal{D}, \mathcal{H}_{\rm f})$. However, by construction $H \# \pi$ takes values in $\mathcal{B}(\mathcal{H}_{\rm f})$ and, by density of $\mathcal{D}$, the same must be true for $\pi \# H$.

We are left to show that $\pi \in M^0_\tau(\varepsilon, \mathcal{B}(\mathcal{H}_{\rm f})) \cap M_\tau(\varepsilon, w, \mathcal{B}(\mathcal{H}_{\rm f}, \mathcal{D}))$. To this end notice that by construction π inherits the τ-equivariance of H, i.e.

$$\pi_j(k - \gamma^*, q) = \tau(\gamma^*)\, \pi_j(k, q)\, \tau(\gamma^*)^{-1}\,.$$

From (6.41) and (6.35) we conclude that for each $\alpha \in \mathbb{N}^{2d}$ and $j \in \mathbb{N}$ one has

$$\|(\partial_z^\alpha \pi_j)(z)\| \leq 2\pi C_{\rm r} \sup_{\zeta \in \Lambda(z_0)} \|(\partial_z^\alpha R_j)(\zeta, z)\|\,, \tag{6.42}$$

where $\|\cdot\|$ stands either for the norm of $\mathcal{B}(\mathcal{H}_{\rm f})$ or for the norm of $\mathcal{B}(\mathcal{H}_{\rm f}, \mathcal{D})$. In order to show that $\pi \in M^\varepsilon_\tau(1, \mathcal{B}(\mathcal{H}_{\rm f}))$ it suffices to consider $z = (k, r) \in B \times \mathbb{R}^d$ since $\tau(\gamma^*)$ is unitary and thus the $\mathcal{B}(\mathcal{H}_{\rm f})$-norm of π is periodic. According to (6.42) we must show that

$$\|(\partial_z^\alpha R_j)(\zeta, z)\|_{\mathcal{B}(\mathcal{H}_{\rm f})} \leq C_{\alpha j} \quad \forall\, z \in \mathcal{U}_{z_0},\, \zeta \in \Lambda(z_0) \tag{6.43}$$

with $C_{\alpha j}$ independent of $z_0 \in B \times \mathbb{R}^d$.

To prove (6.43) we use an induction argument. Assume, by induction hypothesis, that for any $j \leq n$ one has that

$$R_j(\zeta) \in S_\tau(1, \mathcal{B}(\mathcal{H}_{\rm f})) \cap S_\tau(w, \mathcal{B}(\mathcal{H}_{\rm f}, \mathcal{D})) \tag{6.44}$$

uniformly in ζ (in the sense that the Frechet seminorms are bounded by ζ-independent constants). Then, according to Prop. 19, $E_{n+1}(\zeta)$, as defined by (6.37), belongs to $S_\tau(w^2, \mathcal{B}(\mathcal{H}_{\rm f}))$ uniformly in ζ. By τ-equivariance, the norm of $E_{n+1}(\zeta)$ is periodic and one concludes that $E_{n+1}(\zeta) \in S_\tau(1, \mathcal{B}(\mathcal{H}_{\rm f}))$ uniformly in ζ. It follows from (6.38) that (6.44) is satisfied for $j = n + 1$.
We are left to show that (6.44) is fulfilled for $j = 0$. We notice that according to (6.34) one has for all $z \in \mathbb{R}^{2d}$

$$\|R_0(\zeta)\|_{\mathcal{B}(\mathcal{H}_{\rm f})} = \|(H(z) - \zeta)^{-1}\|_{\mathcal{B}(\mathcal{H}_{\rm f})} = \frac{1}{\operatorname{dist}(\zeta, \sigma(H(z)))} \leq \frac{4}{C_{\rm g}}\,.$$

By chain rule,

$$\|(\partial_z R_0)(\zeta, z)\|_{\mathcal{B}(\mathcal{H}_{\rm f})} = \|(R_0(\zeta)(\partial_z H_0) R_0(\zeta))(z)\|_{\mathcal{B}(\mathcal{H}_{\rm f})} \tag{6.45}$$

Since $\partial_z H_0\, R_0(\zeta)$ is a τ-equivariant $\mathcal{B}(\mathcal{H}_{\rm f})$-valued symbol, its norm is periodic and then can be estimated for $z \in B \times \mathbb{R}^d$, getting the required bound. For a general $\alpha \in \mathbb{N}^{2d}$, the norm of $\partial_z^\alpha R_0(\zeta)$ can be bounded in a similar way. This proves that $R_0(\zeta)$ belongs to $S_\tau(1, \mathcal{B}(\mathcal{H}_{\rm f}))$ uniformly in ζ.

On the other hand

$$\begin{aligned}\|R_0(k,r)\|_{\mathcal{B}(\mathcal{H}_{\rm f},\mathcal{D})} &= \|(1+\Delta_x)\,R_0([k]+\gamma^*,r)\|_{\mathcal{B}(\mathcal{H}_{\rm f})} = \|(1+\Delta_x)\,\tau(\gamma^*)R_0([k],r)\tau^{-1}(\gamma^*)\|_{\mathcal{B}(\mathcal{H}_{\rm f})}\\ &\leq C\,\|(1+\gamma^{*2})(1+\Delta_x)\,R_0([k],r)\|_{\mathcal{B}(\mathcal{H}_{\rm f})} \leq C'(1+\gamma^{*2}) \leq 2C'(1+k^2)\end{aligned}$$

where we used the fact that $\|(1+\Delta_x)R_0(z)\|_{\mathcal{B}(\mathcal{H}_{\rm f})}$ is bounded for $z \in B \times \mathbb{R}^d$. The previous estimate and the fact that $\partial_z H_0\ R_0(\zeta) \in S_\tau(1,\mathcal{B}(\mathcal{H}_{\rm f}))$ yield

$$\|(\partial_z R_0)(\zeta,z)\|_{\mathcal{B}(\mathcal{H}_{\rm f},\mathcal{D})} = \|(R_0(\zeta)(\partial_z H_0)R_0(\zeta))(z)\|_{\mathcal{B}(\mathcal{H}_{\rm f},\mathcal{D})} \leq C(1+k^2). \quad (6.46)$$

Higher order derivatives, are bounded by the same argument, yielding that $R_0(\zeta)$ belongs to $S_\tau(w,\mathcal{B}(\mathcal{H}_{\rm f},\mathcal{D}))$ uniformly in ζ. This conclude the induction argument.

From the previous argument it follows moreover that

$$\|(\partial_z^\alpha R_j)(\zeta,z)\|_{\mathcal{B}(\mathcal{H}_{\rm f},\mathcal{D})} \leq C_{\alpha j}\ w(z) \quad \forall\ z \in \mathcal{U}_{z_0},\ \zeta \in \Lambda(z_0) \quad (6.47)$$

with $C_{\alpha j}$ independent of $z_0 \in \mathbb{R}^{2d}$. By (6.42), this imply that $\pi \in M_\tau^\varepsilon(w,\mathcal{B}(\mathcal{H}_{\rm f},\mathcal{D}))$ and concludes the proof.

□

Proof of Proposition 34. From the projector constructed in Lemma 35 one obtains, by resummation, a semiclassical symbol $\pi \in S^\varepsilon(1,\mathcal{H}_{\rm f})$ whose asymptotic expansion is given by $\sum_{j\geq 0}\varepsilon^j\pi_j$. Then, by Weyl quantization, one gets a bounded operator $\widehat{\pi} \in \mathcal{B}(\mathcal{H}_\tau)$ (see Prop. 25) which is an almost-projector, in the sense that

$$\widehat{\pi}^2 = \widehat{\pi} + \mathcal{O}_0(\varepsilon^\infty) \text{ and } \widehat{\pi}^* = \widehat{\pi}.$$

We notice that from Prop. 19 it follows that $H\,\tilde{\#}\,\pi \in S_\tau(w^2,\mathcal{B}(\mathcal{H}_{\rm f}))$. But τ-equivariance implies that the norm is periodic and then $H\,\tilde{\#}\,\pi$ belongs to $S_\tau(1,\mathcal{B}(\mathcal{H}_{\rm f}))$. Then $\pi\,\tilde{\#}\,H = (H\,\tilde{\#}\,\pi)^*$ belongs to the same class, so that $[H,\pi]_{\tilde{\#}} \in S_\tau(1,\mathcal{B}(\mathcal{H}_{\rm f}))$. This *a priori* information on the symbol class, together with Lemma 35.iii, assure that

$$[\widehat{H},\widehat{\pi}] = \mathcal{O}_0(\varepsilon^\infty) \quad (6.48)$$

with the remainder bounded in the $\mathcal{B}(\mathcal{H}_{\rm f})$-norm.

In order to get a true projector, we follow an idea by Nenciu. For ε small enough, let

$$\Pi^\varepsilon := \frac{i}{2\pi}\int_{|\zeta-1|=\frac{1}{2}} (\widehat{\pi}-\zeta)^{-1}\,d\zeta\,. \quad (6.49)$$

Then it follows as in [PST$_1$] that $(\Pi^\varepsilon)^2 = \Pi^\varepsilon$, $\Pi^\varepsilon = \widehat{\pi} + \mathcal{O}_0(\varepsilon^\infty)$ and

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

□

6.3.2 The intertwining unitaries

The Assumption (A_2) is equivalent to the following assumption, which claims for the existence of a fundamental unitary.

Assumption (A_2'). We assume that there exists a projector $\pi_r \in \mathcal{B}(\mathcal{H}_f)$ and a unitary-operator valued map $u_0 : \mathbb{R}^{2d} \to \mathcal{U}(\mathcal{H}_f)$ so that

$$u_0^*(k,r)\,\pi_0(k,r)\,u_0(k,r) = \pi_r \tag{6.50}$$

for any $(k,r) \in \mathbb{R}^{2d}$,

$$u_0(k+\gamma^*,r) = \tau(\gamma^*)^* u_0(k,r), \tag{6.51}$$

and u_0 belong to $S(1,\mathcal{B}(\mathcal{H}_f))$. ♢

Clearly,

$$u_0^*(k+\gamma,r) = u_0^*(k,r)\tau(\gamma). \tag{6.52}$$

An operator valued symbol satisfying (6.51) (resp.6.52) will be called left τ-covariant (resp. right τ-covariant).

To be explicit, according to Assumption (A_2), there exists an orthonormal basis $\{\psi_i(k)\}_{i=1}^m$ of $\mathrm{Ran}P_{\mathcal{I}}(k)$ which is smooth and τ-equivariant with respect to k. Let $\pi_r := \pi_0(k_0,r_0)$ for any fixed point (k_0,r_0). By the gap condition, $\dim\pi_r = \dim P_{\mathcal{I}}(k)$. Then for any orthonormal basis $\{\chi_i\}_{i=1}^m$ for $\mathrm{Ran}\pi_r$, the formula

$$\tilde{u}_0(k,r) := \sum_{i=1}^m |\psi_i(k-A(r))\rangle\langle\chi_i|\,, \tag{6.53}$$

defines a partial isometry which can be extended to a unitary operator $u_0(k,r) \in \mathcal{U}(\mathcal{H}_f)$. The fact that $\{\psi_i(k)\}_{i=1}^m$ spans $\mathrm{Ran}P_{\mathcal{I}}(k)$ implies (6.50), and the τ-equivariance of $\psi_i(k)$ reflects in (6.51).

Viceversa, given u_0 fulfilling Assumption (A_2'), one can check that the formula

$$\psi_i(k-A(r)) := u_0(k,r)\chi_i, \tag{6.54}$$

with $\{\chi_i\}_{i=1}^m$ spanning $\mathrm{Ran}\pi_r$, defines an orthonormal basis for $\mathrm{Ran}P_{\mathcal{I}}(k)$ which satisfies Assumption (A_2).

The goal of this section is to construct a unitary operator which allow us to map the intraband dynamics from $\mathrm{Ran}\Pi^\varepsilon$ to an ε-independent reference space $\mathcal{K}_{\mathrm{ref}} \subset \mathcal{H}_{\mathrm{ref}}$. Since all the twisting of $\mathcal{H}_\tau$ has been absorbed in the τ-equivariant basis $\{\chi_i\}_{i=1}^m$, or equivalently in u_0, the space $\mathcal{H}_{\mathrm{ref}}$ can be chosen to be a space of *periodic* vector-valued functions, i.e.

$$\mathcal{H}_{\mathrm{ref}} := L^2_{\tau\equiv 1}(\mathbb{R}^d,\mathcal{H}_f) \cong L^2(\mathbb{T}^d,\mathcal{H}_f). \tag{6.55}$$

It is convenient to introduce the orthogonal projector $\Pi_{\rm ref} := \hat{\pi}_{\rm r} \in \mathcal{B}(\mathcal{H}_{\rm ref})$ since the effective intraband dynamics can be described in

$$\mathcal{K}_{\rm ref} := {\rm Ran}\Pi_{\rm ref} \cong L^2_{\tau\equiv 1}(\mathbb{R}^d, \mathbb{C}^m) \cong L^2(\mathbb{T}^d, \mathbb{C}^m) \tag{6.56}$$

as it will become apparent later on. Recall that $m = {\rm dim}P_{\mathcal{I}}(k) = {\rm dim}\pi_{\rm r}$.

Proposition 36 (Existence of intertwining unitaries). *Let $\{E_n\}_{n\in\mathcal{I}}$ be an isolated group of bands, see Definition 32, and let Assumptions* ($\rm A_1$) *and* ($\rm A_2'$) *be satisfied. Then there exist a unitary operator $U : \mathcal{H}_{\rm ref} \to \mathcal{H}_\tau$ such that*

$$U^*\,\Pi^\varepsilon\,U = \Pi_{\rm ref} \tag{6.57}$$

and $U = \hat{u} + \mathcal{O}_0(\varepsilon^\infty)$, where $u \asymp \sum_{j\geq 0}\varepsilon^j u_j$ belong to $S^\varepsilon(1, \mathcal{B}(\mathcal{H}_{\rm f}))$, is left τ-covariant at any order and has principal symbol u_0.

Proof. As usual, there are two logical steps.

I. Construction of the symbol. The proof follows step by step the construction given in Chapter 2. Since u_0 is left τ-covariant, one proves by induction that the same holds true for any u_j. Indeed, by referring to the notation in [PST$_1$], one has that

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

with $a_{n+1} = -\frac{1}{2}A_{n+1}$ and $b_{n+1} = [B_{n+1}, \pi_r]$. From the defining equation

$$u^{(n)*} \,\#\, u^{(n)} - 1 = \varepsilon^{n+1}A_{n+1} + \mathcal{O}(\varepsilon^{n+2})$$

and the induction hypothesis, it follows that A_{n+1} is a periodic symbol. Then $w^{(n)} := u^{(n)} + \varepsilon^{n+1}u_0a_{n+1}$ is left τ-covariant. Then the defining equation

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

shows that B_{n+1} is a periodic symbol, and so is b_{n+1}. Then any u_j is left τ-covariant, and in particular there exists a semiclassical symbol $u \asymp \sum_j \varepsilon^j u_j$ so that $u \in S^\varepsilon(1, \mathcal{B}(\mathcal{H}_{\rm f}))$.

II. Quantization. One notices that left τ-covariance is nothing but a special case of (τ_1, τ_2)-equivariance, for $\tau_1 \equiv 1$ and $\tau_2 = \tau^*$. Then from Prop. 26 it follows that the Weyl quantization of u is a bounded operator $\hat{u} \in \mathcal{B}(\mathcal{H}_{\rm ref}, \mathcal{H}_\tau)$ such that:

(i) $\hat{u}^*\hat{u} = 1_{\mathcal{H}_{\rm ref}} + \mathcal{O}_0(\varepsilon^\infty)$ and $\quad \hat{u}\hat{u}^* = 1_{\mathcal{H}_\tau} + \mathcal{O}_0(\varepsilon^\infty)$

(ii) $\hat{u}^* \Pi^\varepsilon \hat{u} = \Pi_{\text{ref}} + \mathcal{O}_0(\varepsilon^\infty)$

We wish now to modify $\hat{u}$ by an $\mathcal{O}_0(\varepsilon^\infty)$-term in order to get a true unitary operator $\tilde{U} \in \mathcal{U}(\mathcal{H}_{\text{ref}}, \mathcal{H}_\tau)$. Let us define

$$\tilde{U} = (\hat{u}\hat{u}^*)^{-\frac{1}{2}} \hat{u} \tag{6.58}$$

Notice that $\hat{u}\hat{u}^*$ is a self-adjoint positive operator which is $\mathcal{O}_0(\varepsilon^\infty)$-close to the identity operator; then $(\hat{u}\hat{u}^*)^{-\frac{1}{2}}$ is well-defined and again $\mathcal{O}_0(\varepsilon^\infty)$-close to the identity operator. Hence (6.58) defines a unitary operator which moreover is $\mathcal{O}_0(\varepsilon^\infty)$-close to $\hat{u}$. Then from (ii) and the boundness of Π^ε and Π_{ref}, it follows that

$$\tilde{U}^* \, \Pi^\varepsilon \, \tilde{U} = \Pi_{\text{ref}} + \mathcal{O}_0(\varepsilon^\infty).$$

Finally, by using Nagy's formula one gets a unitary operator $U \in \mathcal{B}(\mathcal{H}_{\text{ref}}, \mathcal{H}_\tau)$ which *exactly* intertwines Π^ε and Π_{ref} and is $\mathcal{O}_0(\varepsilon^\infty)$-close to $\hat{u}$. □

6.3.3 The effective hamiltonian

The next step in space-adiabatic perturbation theory is to describe the intraband dynamics and to compute an effective hamiltonian for it.

Proposition 37 (Effective hamiltonian for the Bloch electron). *Let $\{E_n\}_{n\in\mathcal{I}}$ be an isolated group of bands and let Assumptions (A_1) and (A_2) be satisfied. Define*

$$H_{\text{eff}} := U^* \, \widehat{\pi} \, H^\varepsilon_{\text{BF}} \, \widehat{\pi} \, U. \tag{6.59}$$

Then $H_{\text{eff}} \in \mathcal{B}(\mathcal{H}_{\text{ref}})$, $[H_{\text{eff}}, \Pi_{\text{ref}}] = \mathcal{O}_0(\varepsilon^\infty)$ and

$$(e^{-iH^\varepsilon_{\text{BF}}t} - U \, e^{-iH_{\text{eff}}t} \, U^*)\Pi^\varepsilon = \mathcal{O}_0(\varepsilon^\infty(1+|t|)). \tag{6.60}$$

Moreover $H_{\text{eff}} = \widehat{h}_{\text{eff}} + \mathcal{O}_0(\varepsilon^\infty)$ with h_{eff} a periodic symbol in $S^\varepsilon_{\tau\equiv 1}(1, \mathcal{B}(\mathcal{H}_{\text{f}}))$ given by a resummation of the formal symbol

$$u^* \, \# \, \pi \, \# \, H \, \# \, \pi \, \# \, u. \tag{6.61}$$

Finally $[\widehat{h}_{\text{eff}}, \Pi_{\text{ref}}] = 0$, i.e. $\widehat{h}_{\text{eff}}$ is exactly diagonal in the splitting of $\mathcal{H}_{\text{ref}}$ induced by Π_{ref}.

Notice that from (6.60) it follows that

$$(e^{-iH^\varepsilon_{\text{BF}}t} - U \, e^{-i\widehat{h}_{\text{eff}}t} \, U^*)\Pi^\varepsilon = \mathcal{O}_0(\varepsilon^\infty|t|). \tag{6.62}$$

This is the crucial fact we will use later on.

In the proof we denote $H^\varepsilon_{\text{BF}}$ as $\widehat{H}$ to emphasize the fact that it is the Weyl quantization of $H \in S_\tau(w, \mathcal{B}(\mathcal{D}, \mathcal{H}_{\text{f}}))$.

Proof. We know *a priori*, by the proof of Prop. 34, that $H \tilde{\#} \pi$ and $\pi \tilde{\#} H$ belong to $S^{\varepsilon}_{\tau}(1, \mathcal{B}(\mathcal{H}_{\rm f}))$. Then, by Theorem 25, $\widehat{H}\,\widehat{\pi} \in \mathcal{B}(\mathcal{H}_{\tau})$ and $\widehat{\pi}\,\widehat{H} \in \mathcal{B}(\mathcal{H}_{\tau})$. In particular, $H_{\rm eff} \in \mathcal{B}(\mathcal{H}_{\rm ref})$. By the intertwining property (6.57) one has

$$H_{\rm eff}\Pi_{\rm ref} = U^*\,\widehat{\pi}\,\widehat{H}\,\widehat{\pi}\,\Pi^{\varepsilon}\,U = U^*\,\widehat{\pi}\,\widehat{H}\,\widehat{\pi}\,U + \mathcal{O}_0(\varepsilon^{\infty}) = \Pi_{\rm ref}H_{\rm eff} + \mathcal{O}_0(\varepsilon^{\infty})$$

where we used the fact that $\widehat{\pi}^2 = \widehat{\pi} + \mathcal{O}_0(\varepsilon^{\infty})$ and the *a priori* estimate to bound the remainder. From (6.59) and the fact that $\Pi^{\varepsilon} = \widehat{\pi} + \mathcal{O}_0(\varepsilon^{\infty})$ it follows that

$$\begin{aligned}
(e^{-i\widehat{H}t} - U\,e^{-iH_{\rm eff}t}U^*\,)\Pi^{\varepsilon} &= (e^{-i\widehat{H}t} - e^{-i\widehat{\pi}\widehat{H}\widehat{\pi}t}\,)\widehat{\pi} + \mathcal{O}_0(\varepsilon^{\infty}) \\
&= -ie^{-i\widehat{H}t}\int_0^t ds\; e^{i\widehat{H}s}\left(\widehat{H} - \widehat{\pi}\widehat{H}\widehat{\pi}\right)e^{-i\widehat{\pi}\widehat{H}\widehat{\pi}s}\widehat{\pi} + \mathcal{O}_0(\varepsilon^{\infty}) \\
&= -ie^{-i\widehat{H}t}\int_0^t ds\; e^{i\widehat{H}s}\left(\widehat{H} - \widehat{\pi}\widehat{H}\widehat{\pi}\right)\widehat{\pi}\,e^{-i\widehat{\pi}\widehat{H}\widehat{\pi}s}\,\widehat{\pi} + \mathcal{O}_0(\varepsilon^{\infty}) \\
&= \mathcal{O}_0(\varepsilon^{\infty}(1+|t|)).
\end{aligned}$$

where we used that $\widehat{H}\widehat{\pi} - \widehat{\pi}\widehat{H}\widehat{\pi} = \mathcal{O}_0(\varepsilon^{\infty})$ as a consequence of (6.48).
From the fact that $H\#\,\pi \in M^{\varepsilon}_{\tau}(1, \mathcal{B}(\mathcal{H}_{\rm f}))$, the comment following Prop. 24 and the τ-covariance of u it follows that $h_{\rm eff} \in S^{\varepsilon}_{\tau\equiv 1}(1, \mathcal{B}(\mathcal{H}_{\rm f}))$. Since $h_{\rm eff}$ and $u^* \,\tilde{\#}\, \pi \,\tilde{\#}\, H \,\tilde{\#}\, \pi \,\tilde{\#}\, u$ have, by definition, the same asymptotic expansion in ε, one concludes that $\widehat{h}_{\rm eff} = \hat{u}^*\,\hat{\pi}\,\widehat{H}\,\hat{\pi}\,\hat{u} + \mathcal{O}_0(\varepsilon^{\infty})$. Then, by the *a priori* estimate, one obtains $H_{\rm eff} = \widehat{h}_{\rm eff} + \mathcal{O}_0(\varepsilon^{\infty})$. Finally, by the fact that

$$u^* \,\#\, \pi \,\#\, H \,\#\, \pi \,\#\, u = \pi_{\rm r} \,\#\, u^* \,\#\, H \,\#\, u \,\#\, \pi_{\rm r} = \pi_{\rm r}\,(u^* \,\#\, \pi \,\#\, H \,\#\, \pi \,\#\, u)\,\pi_{\rm r}$$

one concludes that $\widehat{h}_{\rm eff} = \Pi_{\rm ref}\widehat{h}_{\rm eff}\Pi_{\rm ref}$. In particular, $\widehat{h}_{\rm eff}$ is diagonal in the splitting induced by $\Pi_{\rm ref}$. □

Since $[\widehat{h}_{\rm eff}, \Pi_{\rm ref}] = 0$, the effective hamiltonian will be regarded, without differences in notation, either as an element of $\mathcal{B}(\mathcal{H}_{\rm ref})$ or as an element of $\mathcal{B}(\mathcal{K}_{\rm ref})$. Analogously, $h_{\rm eff}$ can be confused with $\pi_{\rm r}h_{\rm eff}\pi_{\rm r}$ and regarded as a $\mathcal{B}(\mathbb{C}^m)$-valued symbol.

6.3.4 Leading order expansions and physical consequences

The next step in adiabatic perturbation theory consists in explicitly compute the symbol $h_{\rm eff}(k, r)$ of the effective hamiltonian.

We first consider the special but most relevant case of an isolated m-fold degenerate eigenvalue, i.e. $E_n(k) \equiv E(k)$ for every $n \in \mathcal{I}$, $|\mathcal{I}| = m$. Recall that in this special case Assumption (A_2) is equivalent to the existence of an orthonormal system of smooth and τ-equivariant Bloch functions relative to the

eigenvalue $E_*(k)$. The part of u_0 intertwining π_0 and π_r is given by equation (6.53) where $\psi_i(k)$ are now Bloch functions, i.e. eigenvectors of $H_\mathrm{per}(k)$ relative to the eigenvalue $E_*(k)$.

In the following proposition, h_eff is identified with $\pi_\mathrm{r} h_\mathrm{eff} \pi_\mathrm{r}$ and regarded as a $\mathcal{B}(\mathbb{C}^m)$-valued symbol. We consider the matrix elements

$$h_\mathrm{eff}(k,r)_{\alpha\beta} := \langle \chi_\alpha, h_\mathrm{eff}(k,r)\chi_\beta \rangle \tag{6.63}$$

for $\alpha, \beta \in \{1, \ldots, m\}$. For sake of simplicity, the result is stated only for $d = 3$.

Proposition 38. *Let $E(k)$ an isolated m-fold degenerate eigenvalue and let Assumptions (A_1) and (A_2) hold true. Let $d = 3$. Then*

$$h_0(k,r)_{\alpha\beta} = (E(k - A(r)) + W(r))\delta_{\alpha\beta} \tag{6.64}$$

and

$$\begin{aligned} h_1(k,r)_{\alpha\beta} &= (\nabla W(r) - (v(\tilde{k}) \wedge B(r))) \cdot A_\mathrm{Berry}(\tilde{k})_{\alpha\beta} \\ &- \frac{i}{2}\, B(r) \cdot \langle \nabla\psi_\alpha(\tilde{k}),\ \wedge (H_\mathrm{per}(\tilde{k}) - E(\tilde{k}))\nabla\psi_\beta(\tilde{k}) \rangle_{\mathcal{H}_\mathrm{f}} \end{aligned} \tag{6.65}$$

where we abbreviated $B = \mathrm{d}A$, $\tilde{k} = k - A(r)$, $v(k) = \nabla E(k)$ and

$$A_\mathrm{Berry}(k)_{\alpha\beta} = i\langle \psi_\alpha(k), \nabla\psi_\beta(k) \rangle. \tag{6.66}$$

Proof. Equation (6.64) follows immediately from the fact that $h_0 = u_0^* H_0\, u_0$ and that ψ_α are Bloch functions. As for h_1, by the general argument developed in [PST$_1$, Sec. 5.2] it follows that

$$\pi_\mathrm{r} h_1 \pi_\mathrm{r} = -\frac{i}{2}\, \pi_\mathrm{r}(u_0^*\{H_0, u_0\} - u_0^*\{u_0, E_\mathrm{r}\})\pi_\mathrm{r}, \tag{6.67}$$

where $E_\mathrm{r}(k,r) = E(k - A(r)) + W(r)$ and $\{A, B\} := \nabla_r A \cdot \nabla_k B - \nabla_k A \cdot \nabla_r B$ are the Poisson brackets. To extract the Berry connection it is convenient to rewrite (6.67) as

$$\pi_\mathrm{r} h_1 \pi_\mathrm{r} = -\frac{i}{2}\, \pi_\mathrm{r}(u_0^*\{H_\mathrm{per} - E, u_0\} + 2\, u_0^*\{E_\mathrm{r}, u_0\})\pi_\mathrm{r}. \tag{6.68}$$

Inserting (6.53) and performing a straightforward computation the second term gives the first term in (6.65) while the first term contributes to the $\alpha\beta$ matrix element with

$$\frac{i}{2} \sum_{j,l=1}^{d} (\partial_j A_l - \partial_l A_j)(r)\ \ \langle \psi_\alpha(\tilde{k}), \partial_l (H_\mathrm{per} - E)(\tilde{k})\ \partial_j \psi_\beta(\tilde{k}) \rangle_{\mathcal{H}_\mathrm{f}}. \tag{6.69}$$

The derivative on $(H_{\rm per} - E)$ can be moved to the first argument of the inner product by noticing that

$$0 = \nabla\langle\psi_\alpha, (H_{\rm per} - E)\phi\rangle = \langle\nabla\psi_\alpha, (H_{\rm per} - E)\phi\rangle + \langle\psi_\alpha, \nabla(H_{\rm per} - E)\phi\rangle \quad (6.70)$$

since ψ_α is in the kernel of $(H_{\rm per} - E)$. A rearrangement of the sum in the indexes j, l yields (6.65), concluding the proof. □

In the general case in which crossings of eigenvalues inside the relevant band are presents, the previous method still allow to compute the symbol $h_{\rm eff}(k, r)$ of the effective hamiltonian at the leading orders. However, in general, the principal symbol $h_0(k, r)$ is not a multiple of the identity matrix as in (6.64). As a consequence, the pseudodifferential operator $\hat{h}_{\rm eff}$ does not allow a convenient semiclassical limit, i.e. expectation values of time-evolved observables cannot be approximated by using a classical hamiltonian flow (see Sec. 6.3.5). This correspond, from the physical viewpoint, to the well-known fact that the dynamics at the crossing points is essentially not classical.

6.3.5 Semiclassical observables

All over this section it is assumed that Assumptions (A_1) and (A_2) hold true and that the relevant band consist of an isolated m-fold degenerate eigenvalue $E(k)$.

The ultimate goal of the semiclassical model is to approximate the expectation values of a suitable class of observables with quantities which can be computed by the knowledge of the hamiltonian flow $\Phi^t_{\rm sc}$ induced by the semiclassical hamiltonian $H_{\rm sc}(k, r) = E(k - A(r)) + W(r)$. Clearly, not any quantum observable can be approximated by the semiclassical model, so we have to focus on a suitable subclass. This class depend on the degree of approximation we are looking for. A convenient choice can be the following one.

Definition 39 ($\mathcal{O}(\varepsilon^\nu)$-semiclassical observables in BF representation). *Let $\nu \in \mathbb{N} \cup \{+\infty\}$. An operator $B \in \mathcal{B}_{\rm sa}(\mathcal{H}_\tau)$ is called a $\mathcal{O}(\varepsilon^\nu)$-semiclassical observable if there exists a semiclassical symbol $b \in S^\varepsilon_\tau(1, \mathcal{B}(\mathcal{H}_{\rm f}))$ such that*

$$B = b(k, i\nabla^\tau_k) + \mathcal{O}_0(\varepsilon^\nu).$$

The case of unbounded self-adjoint operators can be recovered by considering the spectral measure associated to them. In this spirit, the hamiltonian $H^\varepsilon_{\rm BF}$ and the "not-electrostatic energy" $H_{\rm per}(k - A(i\nabla^\tau_k))$ can be regarded as $\mathcal{O}(\varepsilon^\infty)$-semiclassical observables. Notice moreover that we do not assume that $[b, \pi]_{\tilde{\#}} = \mathcal{O}(\varepsilon^\nu)$ (the reason will be clear later on) so that this definition is independent from the hamiltonian and from the choice of the relevant band. The

price to pay is that a semiclassical observable can be "semiclassically estimated" only on a suitable class of states.

A natural question is the following: how do semiclassical observables look like in the original representation? A partial answer is given by the following result.

Proposition 40 ($\mathcal{O}(\varepsilon^\nu)$-semiclassical observables in original repr.). *Let $B \in \mathcal{B}_{\rm sa}(\mathcal{H}_\tau)$ a $\mathcal{O}(\varepsilon^\nu)$-semiclassical observable whose symbol is a multiple of $1_{\mathcal{H}_{\rm f}}$. Let $A := \mathcal{U}^* B \mathcal{U} \in \mathcal{B}(\mathcal{H})$. Then there exist a scalar semiclassical symbol $a \in S^\varepsilon(1, \mathbb{C})$, with the property that*

$$a(q, p + \gamma^*) = a(q, p) \qquad \forall \gamma * \in \Gamma^*, \tag{6.71}$$

such that

$$A = a(x, -i\nabla_x) + \mathcal{O}_0(\varepsilon^\nu).$$

Moreover, denoting by $\mathcal{F}$ the Fourier transform, one has that $\mathcal{F}a$ is supported over $\mathbb{R}^d \times \Gamma$ and formally

$$(\mathcal{F}a)(\eta, \gamma) = (\mathcal{F}b)(\gamma, \eta) \qquad \forall (\eta, \gamma) \in \mathbb{R}^d \times \Gamma \tag{6.72}$$

Clearly, equation (6.72) has nothing to do with pointwise values and is just a shorthand to say that $\mathcal{F}a$ agrees with $\mathcal{F}b$ after exchanging the order of the variables.

Example 41. Here some interesting and non trivial example. Physical discussion... ♢

Remark 42. An analogous statement *cannot* be true for a general operator-valued τ-equivariant symbol. For example, the symbol $b(k, r) := H_{per}(k - A(r))$ is τ-equivariant. However, the corresponding operator in the original representation is

$$A = \mathcal{U}^{-1} b(k, i\varepsilon\nabla_k^\tau)\mathcal{U} = -\frac{1}{2}(-i\nabla_x - A(\varepsilon x))^2 + V_\Gamma(x) \tag{6.73}$$

which cannot be written as $a(\varepsilon x, -i\nabla_x)$ for any symbol $a(q, p)$ Γ^*-periodic in the second variable. ♢

Proof. Since the class $\mathcal{O}_0(\varepsilon^\nu)$ is invariant under unitary equivalence one has just to prove that $b(k, i\varepsilon\nabla_k^\tau)$ corresponds to $a(\varepsilon x, -i\nabla_x)$. We first recall that for any $a \in S(1, \mathbb{C})$ and any $\psi \in L^2(\mathbb{R}^d)$ one has that

$$(a(\varepsilon x, -i\nabla_x)\psi)(x) = \int_{\mathbb{R}^{2d}} {\rm d}\eta{\rm d}\xi (\mathcal{F}a)(\eta, \xi)\, e^{i\varepsilon(\eta\cdot\xi)/2} e^{i\varepsilon\eta\cdot x}\psi(x + \gamma). \tag{6.74}$$

On the other side, let $(\mathcal{U}\psi)(k,y) =: \varphi(k,y)$. Then, since b is Γ^*-periodic in the first variable, one has

$$(b(k, i\varepsilon\nabla_k^\tau)\varphi)(k,y) = \sum_{\gamma\in\Gamma} \int_{\mathbb{R}^d} \mathrm{d}\eta (\mathcal{F}b)(\gamma,\eta)\ e^{-i\varepsilon(\eta\cdot\gamma)/2} e^{i\gamma\cdot k} \varphi(k-\varepsilon\eta, y). \tag{6.75}$$

This will be made rigorous later on. For the moment we notice that, since $\mathcal{F}b$ is a multiple of the identity, one has

$$\begin{aligned} &(\mathcal{U}^{-1} b(k, i\varepsilon\nabla_k^\tau)\varphi)(x) = \qquad\qquad (6.76)\\ &= \sum_{\gamma\in\Gamma} \int_B \mathrm{d}k \int_{\mathbb{R}^d} \mathrm{d}\eta (\mathcal{F}b)(\gamma,\eta)\ e^{ik\cdot x} e^{-i\varepsilon(\eta\cdot\gamma)/2} e^{i\gamma\cdot k} \varphi(k-\varepsilon\eta, [x]) \\ &= \sum_{\gamma\in\Gamma} \int_{\mathbb{R}^d} \mathrm{d}\eta (\mathcal{F}b)(\gamma,\eta) e^{i\varepsilon(\eta\cdot\gamma)/2} e^{i\varepsilon\eta\cdot x} \int_B \mathrm{d}k\ e^{i(k-\varepsilon\eta)\cdot(x+\gamma)} \varphi(k-\varepsilon\eta,[x]). \end{aligned}$$

The τ-equivariance of φ implies that the function $f(k,y) := e^{ik\cdot y}\varphi(k,[y])$ is exactly periodic in the first variable. Then the integral in $\mathrm{d}k$ can be shifted by an arbitrary amount, so that

$$\int_B \mathrm{d}k\ e^{i(k-\varepsilon\eta)\cdot(x+\gamma)} \varphi(k-\varepsilon\eta,[x]) = \int_B \mathrm{d}k\ e^{ik\cdot(x+\gamma)} \varphi(k,[x+\gamma]) = \psi(x+\gamma)$$

Inserting this expression in the last line of (6.76) and comparing with (6.74) one concludes the proof. □

As pointed out, we want to approximate the expectation values of the time-evolved operator $B(t) := \exp(iH_{\mathrm{BF}}^\varepsilon t)\ B\ \exp(-iH_{\mathrm{BF}}^\varepsilon t)$ on a state $\psi \in \mathrm{Ran}\Pi^\varepsilon$. More generally, let ρ any density operator in $\mathcal{B}(\mathcal{H}_\tau)$ such that $\Pi^\varepsilon\rho = \rho = \rho\Pi^\varepsilon$. Then the expectation value $\mathrm{Tr}_{\mathcal{H}_\tau}(B(t)\rho)$ can be approximated, uniformly in time and in ρ, in the following way:

(i) consider the symbol $c_0 := \pi_{\mathrm{r}}\, u_0^* b_0 u_0\, \pi_{\mathrm{r}} \in S_{\tau\equiv 1}(1, \mathcal{B}(\mathbb{C}^m))$,

(ii) define

$$c_t(k,r) := D^*(k,r,t)\, c_0(\Phi_{\mathrm{sc}}^t(k,r))\, D(k,r,t) \tag{6.77}$$

where $D(\cdot,t)$ is the solution of the Cauchy problem

$$\partial_t D(k,r,t) = -ih_1(\Phi_{\mathrm{sc}}^t(k,r)) D(k,r,t) \tag{6.78}$$

with initial datum $D(k,r,0) \equiv 1$,

(iii) define $C(t) := c_t(k, i\nabla_k^{\mathrm{per}})$ acting in $\mathcal{H}_{\mathrm{ref}}$,

(iv) then $\mathrm{Tr}_{\mathcal{H}_{\mathrm{ref}}}(C(t)U^*\rho U)$ approximate $\mathrm{Tr}_{\mathcal{H}_\tau}(B(t)\rho)$.

The precise sense of the approximation is made clear in the following proposition.

Proposition 43. *Let $B \in \mathcal{B}(\mathcal{H}_\tau)$ an $\mathcal{O}(\varepsilon)$-semiclassical observable and $B(t) := \exp(iH^\varepsilon_{\mathrm{BF}}t)\ B\ \exp(-iH^\varepsilon_{\mathrm{BF}}t)$. Let be ρ a traceclass operator in $\mathcal{H}_\tau$ with $\mathrm{Tr}(\rho) = 1$, such that $\Pi^\varepsilon\rho = \rho = \rho\Pi^\varepsilon$. Let be $C(t)$ defined as above. Then for any $T < +\infty$ there exist a constant C_T such that*

$$|\mathrm{Tr}_{\mathcal{H}_\tau}(B(t)\ \rho) - \mathrm{Tr}_{\mathcal{H}_{\mathrm{ref}}}(C(t)U^*\rho U)| \leq \varepsilon\, C_T \tag{6.79}$$

for every $t \in [-T, T]$. The constant C_T is independent from ρ. In particular, it is part of the statement that the classical flow Φ^t_{sc} generated by H_{sc} and the solution of the Cauchy problem (6.77) exist globally in time and that c_t belong to $S_{\tau\equiv 1}(1, \mathcal{B}(\mathbb{C}^m))$ for every $t \in \mathbb{R}$.

The proof of the proposition is a combination of the usual first-order Egorov-type theorem and the following lemma, which hold true to any order of approximation.

Lemma 44. *Let B any operator in $\mathcal{B}(\mathcal{H}_\tau)$ and $B(t) := \exp(iH^\varepsilon_{\mathrm{BF}}t)\ B\ \exp(-iH^\varepsilon_{\mathrm{BF}}t)$. Let ρ as in the previous proposition and $C(t)$ any $\mathcal{B}(\mathcal{H}_{\mathrm{ref}})$-valued function. Then*

$$\begin{aligned} &|\mathrm{Tr}_{\mathcal{H}_\tau}(B(t)\ \rho) - \mathrm{Tr}_{\mathcal{H}_{\mathrm{ref}}}(C(t)U^*\rho U)| \ \leq \\ &\leq \ \|\Pi_{\mathrm{ref}}(e^{i\hat{h}_{\mathrm{eff}}t}\Pi_{\mathrm{ref}}UBU^*\Pi_{\mathrm{ref}}e^{-i\hat{h}_{\mathrm{eff}}t} \ - \ C(t))\Pi_{\mathrm{ref}}\|_{\mathcal{B}(\mathcal{H}_{\mathrm{ref}})} + \mathcal{O}(\varepsilon^\infty|t|) \end{aligned}$$

where the remainder is independent from ρ.

Proof. Let $\rho' = U^*\rho U$ so that $\rho' = \Pi_{\mathrm{ref}}\rho'\Pi_{\mathrm{ref}}$. By the invariance of the trace under unitary equivalence and the ciclic property one gets

$$\begin{aligned} |\mathrm{Tr}_{\mathcal{H}_\tau}(B(t)\ \rho) \ - \ &\mathrm{Tr}_{\mathcal{H}_{\mathrm{ref}}}(C(t)U^*\rho U)| = |\mathrm{Tr}_{\mathcal{H}_{\mathrm{ref}}}((U^*B(t)U - C(t))\rho')| \\ = \ &|\mathrm{Tr}_{\mathcal{H}_{\mathrm{ref}}}(\Pi_{\mathrm{ref}}(U^*e^{iH^\varepsilon_{\mathrm{BF}}t}Be^{-iH^\varepsilon_{\mathrm{BF}}t}U - C(t))\Pi_{\mathrm{ref}}\rho')| \\ \leq \ &\|\Pi_{\mathrm{ref}}(U^*\Pi^\varepsilon e^{iH^\varepsilon_{\mathrm{BF}}t}Be^{-iH^\varepsilon_{\mathrm{BF}}t}\Pi^\varepsilon U - C(t))\Pi_{\mathrm{ref}}\|_{\mathcal{B}(\mathcal{H}_{\mathrm{ref}})}. \end{aligned}$$

where we used the intertwining property (6.57). Inserting (6.62) one gets that

$$\begin{aligned} \Pi_{\mathrm{ref}}(U^*\Pi^\varepsilon B(t)\Pi^\varepsilon U \ - \ &C(t))\Pi_{\mathrm{ref}} = \\ = \ &\Pi_{\mathrm{ref}}(\Pi_{\mathrm{ref}}e^{i\widehat{h}_{\mathrm{eff}}t}U^*BUe^{-i\widehat{h}_{\mathrm{eff}}t}\Pi_{\mathrm{ref}} - C(t))\Pi_{\mathrm{ref}} + \mathcal{O}_0(\varepsilon^\infty|t|) \\ = \ &\Pi_{\mathrm{ref}}(e^{i\hat{h}_{\mathrm{eff}}t}\Pi_{\mathrm{ref}}UBU^*\Pi_{\mathrm{ref}}e^{-i\hat{h}_{\mathrm{eff}}t} - C(t))\Pi_{\mathrm{ref}} + \mathcal{O}_0(\varepsilon^\infty|t|) \end{aligned}$$

where we used that $[e^{-i\widehat{h}_{\mathrm{eff}}t}, \Pi_{\mathrm{ref}}] = \mathcal{O}_0(\varepsilon^\infty|t|)$. □

The claim of Prop.43 follows easily by noticing that $\Pi_{\rm ref} U B U^* \Pi_{\rm ref} = \hat{\pi}_{\rm r} \hat{u}^* \hat{b} \hat{u} \hat{\pi}_{\rm r} + \mathcal{O}_0(\varepsilon^\infty)$ and applying one of the usual formulations of first order Egorov theorem (see, for example, [PST$_1$, Theorem 6.1]).

Example 45. As an easy but relevant application, one can show that the physical macroscopic velocity is given, at the leading order, by $\tilde{v}(k,r) := \nabla E_{\rm r}(k - A(r))$. This result has been implicitly used in the physical interpretation of the effective hamiltonian (6.28).

Higher order estimates on the expectation values of semiclassical observables can be obtained by using Lemma 44 and an higher-order version of Egorov theorem for *matrix*-valued symbols, as developed, for example, in [Iv].

Chapter 7

Conclusions and perspectives

At this point the reader should be convinced, I hope, that the space-adiabatic approach gives a powerful and general theory which can be applied to a wide range of physically interesting problems in which a separation of time-scales appears. Moreover, we wish to underline the following points:

- the space-adiabatic perturbation theory yields a **model-independent technique** which is, in our opinion, vastly superior to a case by case study.
- in this approach, all the degrees of freedom are **quantum mechanical**, and the main results are formulated in terms of operators over the full Hilbert space $\mathcal{H}$.
- as a consequence, in this approach the **adiabatic decoupling**, a purely quantum mechanical phenomenon based on separation of time-scales, and the **semiclassical limit** are carefully distinguished. In other approaches (references...) the two limits are mixed.
- all the estimates are given in term of the norm of bounded operators over $\mathcal{H}$, so that the estimates are **uniform** with respect to the initial state of the system. Moreover, the use of techniques based on Weyl calculus, allow us to obtain an abiabatic decoupling up to an $\mathcal{O}(\varepsilon^\infty)$**-error**, a result which is impressively better than what can be proved by techniques based on "classical" operator theory.
- last but not least, the theory yields a **perturbation scheme** which allow us to compute the effective hamiltonian to, in principle, any order in ε. Unfortunately, computational effort prevents to go far beyond the first two orders.

As far as applications are concerned, in the present thesis we already give a wide range of applications, including:

Ex.1 Molecular physics. In Sec. 2.4.3 we computed the first order correction to the Born-Oppenheimer approximation, showing that it contains a generalized Berry's connection.

Ex.2.2 Dirac electron. In Ch. 3 we obtained the leading order term and the first order correction in the expansion of the effective hamiltonian. Moreover we obtained the first rigorous deduction of the BMT equation, an equation derived by Bargmann, Michel and Telegdi in 1959 [BMT], on purely classical grounds, as the simplest Lorentz-covariant equation for a classical spin (i.e. a vector in $S^2 \subset \mathbb{R}^3$). The BMT equation has been used for years, until the discovery of particle traps, to compute the anomalous magnetic moment of the electron from experimental data. Therefore, the experimental test of the most outstanding prediction of QED, namely the anomalous g-factor, relied on BMT equation.

Ex.2.3 Pauli-Fierz electron. We obtain in Ch. 4, for the moment at a pre-mathematical level, an effective hamiltonian for the dynamics of the dressed electron in non-relativistic QED. The first order correction gave us the opportunity to obtain a non-perturbative definition of the g-factor.

Ex.4 Bloch electron. The most impressive application of space-adiabatic perturbation theory is probably the case of an electron in a crystal. In Ch.6 we obtained the first rigourous proof of the **Peierl's substituition**, widely used in solid state physics. Moreover, Prop. 38 gives the first order correction to the Peierl' s substitution, whose physical meaning is still to be explored.

The realm of possible future applications is very rich too. First of all, the general scheme could be applied to the constrained quantum motion, as mentioned in the introduction. A second relevant application is the case of the magnetic Bloch electron, i.e. an electron moving in a periodic crystal potential with an additional *strong and constant* magnetic field superimposed. This case, which is relevant for a dynamical understanding of the quantum Hall effect, fits perfectly in the theory formulated in Ch. 5 and 6. However, in the case of a magnetic Bloch electron, Assumption (A_2) (see Sec. 6.3), is generically violated. Therefore one should probably introduce a reference space $\mathcal{H}_{\text{ref}}$ consisting of sections of a suitable Hilbert space bundle, which incorporates the intrinsic twisting of the bundle pointwise defined by $\pi_0(q,p)$ (see Sec. 6.3).

Finally, I wish to outline a possible long-term application of space-adiabatic theory. Indeed, if a rigorous formulation of QED would be available, one could try to prove that the N-electrons sector of the theory is adiabatically decoupled from the remaining sectors, provided that the initial state is such that all the

velocities and accelerations of the electrons are uniformly bounded, in some suitable sense (see [Te] for a similar condition in a different context). Since a rigorous formulation of QED seems far from being available, for the moment these ideas can only be tested on some toy-model, as for example a low-dimensional QFT.

Apart from other possible applications to physically relevant models, the theory can be further developed along three main directions:

- **exponentially small errors.** Assuming analyticity of the symbol of the hamiltonian, one could prove, by using a technique analogous to the one used in [NeSo], that the interband transitions are suppressed up to terms of order $e^{-\frac{C}{\varepsilon}}$, then improving our $\mathcal{O}(\varepsilon^\infty)$-estimates. One cannot expect to go beyond exponentially small errors, since better estimates would be in contrast with physical expectations. Although important from a mathematical viewpoint, exponentially small estimates are not so relevant from the physical viewpoint, since the relevant physical effects depend on the leading orders expansion of the effective hamiltonian.

- **adiabatic decoupling without gap.** As previously pointed out, it is crucial for space-adiabatic perturbation theory that the relevant band is uniformly separated from the remainder of the spectrum by a finite energy gap. However, there are examples, as the massless Nelson model or the massless Pauli-Fierz model, in which the relevant band consist of a single eigenvalue at the bottom of the absolutely continuous spectrum. In a recent paper on the massless Nelson model [Te_2] it has been shown, by using methods of operator theory, that even in this case the adiabatic decoupling holds true up to $\mathcal{O}(\varepsilon\sqrt{\ln(1/\varepsilon)})$-errors. Moreover, the effective hamiltonian in [Te_2] coincide, up to the first order, with the one obtained by formally using the perturbation scheme outlined in Sec. 2.4.2. Further research in this direction seems to be very interesting.

- **crossing of eigenvalues.** Another natural question is what happens when the relevant energy band crosses another energy band. As pointed out, our results can be generalized to the case in which a *local* gap condition is fulfilled, and then the adiabatic decoupling holds true up to times of the order of the *classical hitting time*, which can be roughly estimated as the time at which the support of the initial wavefunction, evolved according to the classical hamiltonian flow, hits the crossing manifold. But, despite of this fact, it is very interesting, both from the mathematical and the physical viewpoint, to understand what happens when the support of the wavefunction hits the crossing manifold. Pioneering work in this direction has been done in [Ha_2] by using gaussian wave-packets. More recent results

are obtained in [FeGe] and [FeLa] by using techniques related to Wigner measures. Further progress in this direction would be of major interest.

Appendix A

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 $\mathcal{H} = L^2(\mathbb{R}^d) \otimes \mathcal{H}_{\rm f}$, where $L^2(\mathbb{R}^d)$ is the state space for the slow degrees of freedom and $\mathcal{H}_{\rm f}$ 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 $\mathcal{B}(\mathcal{H}_{\rm f})$-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 $\mathcal{B}(\mathcal{H}_{\rm f})$-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 $\mathcal{S}(\mathbb{R}^d, \mathcal{E})$, $L^p(\mathbb{R}^d, \mathcal{E})$, with the obvious meaning. Note that, in the special case where $\mathcal{E} = \mathcal{H}_{\rm f}$ is an Hilbert space, one has $L^2(\mathbb{R}^d, \mathcal{H}_{\rm f}) \cong L^2(\mathbb{R}^d) \otimes \mathcal{H}_{\rm f}$. The space of the bounded operators on $\mathcal{E}$ will be denoted as $\mathcal{B}(\mathcal{E})$.

A.1 Weyl quantization

Let A be a $\mathcal{B}(\mathcal{H}_{\rm f})$-valued rapidly decreasing smooth function on $\mathbb{R}^{2d}$, i.e. $A \in \mathcal{S}(\mathbb{R}^{2d}, \mathcal{B}(\mathcal{H}_{\rm f}))$. 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 $\mathcal{B}(\mathcal{H}_{\rm f})$-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 $e^{i(\eta\cdot\widehat{q}+\xi\cdot\widehat{p})}\otimes 1_{\mathcal{H}_{\rm f}}$ 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

$$\left(e^{i(\eta\cdot\widehat{q}+\xi\cdot\widehat{p})}\psi\right)(x) = e^{i\varepsilon(\eta\cdot\xi)/2}e^{i\eta\cdot x}\psi(x+\varepsilon\xi) \qquad \text{for } \psi\in L^2(\mathbb{R}^d). \tag{A.1}$$

Thus

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

and, in particular,

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

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

Substituting (A.1) in (A.2) one obtains that for every $\psi\in\mathcal{S}(\mathbb{R}^d,\mathcal{H}_{\rm f})$

$$(\widehat{A}\psi)(x) = \frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^{2d}} A(\tfrac{1}{2}(x+y),\xi)\, e^{i\xi\cdot(x-y)/\varepsilon}\,\psi(y)\ d\xi dy, \tag{A.3}$$

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

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

Taking (A.3) as a definition, the Weyl quantization can be extended to much larger classes of **symbols** $A(q,p)$.

Definition 46. *A function $A\in C^\infty(\mathbb{R}^{2d},\mathcal{B}(\mathcal{H}_{\rm f}))$ belongs to the symbol class $S^m_\rho(\mathcal{B}(\mathcal{H}_{\rm f}))$ (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*

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

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

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

$$\|A\|^{(m)}_k = \sup_{|\alpha|+|\beta|\le k}\ \sup_{q,p\in\mathbb{R}^d}\langle p\rangle^{-m+\rho|\beta|}\left\|(\partial_q^\alpha\partial_p^\beta A)(q,p)\right\|_{\mathcal{B}(\mathcal{H}_{\rm f})}\,, \qquad k\in\mathbb{N}. \tag{A.4}$$

The following result is proved exactly as in the scalar case, cf. also [GMS].

Proposition 47. *Let $A \in S^m_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$, then $\widehat{A}$ given trough (A.3) maps $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_\mathrm{f})$ continuously into itself.*

Since $A \in S^m_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ implies $A^* \in S^m_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$, the previous result allows to extend $\widehat{A}$ to a continuous map 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 $\rho \geq \rho'$.

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

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

it is a Banach space.

Proposition 48. (Calderon-Vaillancourt) *There exists a constant $C_d < \infty$ such that for every $A \in C^{2d+1}_\mathrm{b}(\mathbb{R}^{2d}, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ one has*

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

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 $S^0(\mathcal{B}(\mathcal{H}_\mathrm{f}))$.

A.2 The Weyl-Moyal product

Next we consider the composition of symbols. 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 49. *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 50. *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*

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

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

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

Similar bounds on derivatives can be obtained by noticing that

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

and applying the chain rule. □

The crucial result for pseudodifferential calculus is the following. One can define an associative product in the space of classical symbols which corresponds to the composition of the operators. Given $A \in S^{m_1}_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ and $B \in S^{m_2}_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ we know that $\widehat{A}$ and $\widehat{B}$ 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 one can show that there exists a unique ε-dependent symbol $\mathrm{Symb}(\widehat{A}\widehat{B}) =: A \,\tilde{\#}\, B \in S^{m_1+m_2}_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ 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. For the proof of the following proposition in the operator valued case we refer again to [GMS].

Proposition 51. *Let $A \in S^{m_1}_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ and $B \in S^{m_2}_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$, then $\widehat{A}\widehat{B} = \widehat{C}$ with $C \in S^{m_1+m_2}_\rho(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ given through*

$$C(q,p) = \exp\left(\frac{i\varepsilon}{2} (\nabla_p \cdot \nabla_x - \nabla_\xi \cdot \nabla_q) \right) (A(q,p)\, B(x,\xi))\Big|_{x=q,\xi=p} =: (A \,\tilde{\#}\, B)(q,p) . \tag{A.5}$$

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 (A.5) 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 52. *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*

$$\left\| A_\varepsilon - \sum_{j=0}^{n-1} \varepsilon^j A_j \right\|_k^{(m-n\rho)} \leq C_{n,k}\, \varepsilon^n \,, \tag{A.6}$$

where $\|\ldots\|_k^{(m)}$ is the k-th Fréchet semi-norm in S^m_ρ, introduced in (5.1).

One calls A_0 and A_1 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 (A.6) 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 53. *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 54. *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 $A \,\tilde{\#}\, B \in S^{m_1+m_2}_\rho(\varepsilon)$ has an asymptotic expansion given by*

$$\left(A \,\tilde{\#}\, B\right)_k (q,p) = (2i)^{-k} \sum_{|\alpha|+|\beta|+j+l=k} \frac{(-1)^{|\alpha|}}{|\alpha|!|\beta|!} \left((\partial_q^\alpha \partial_p^\beta A_j)(\partial_p^\alpha \partial_q^\beta B_l)\right)(q,p) \tag{A.7}$$

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

$$\{A, B\} = \sum_{j=1}^{d} \frac{\partial A}{\partial p_j}\frac{\partial B}{\partial q_j} - \frac{\partial A}{\partial q_j}\frac{\partial B}{\partial p_j}. \tag{A.8}$$

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 (A.7) 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 (A.7) 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 (A.7) 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. 54) 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

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

If $\rho > 0$ we obtain that definitely $m_1 + m_2 - n\rho \lneqq 0$ for some $n \in \mathbb{N}$ and then Prop. 48 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 $OPS_\rho^{-\infty} := \cap_{m\in\mathbb{R}} OPS_\rho^m$) 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

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

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 $[A_\varepsilon, B_\varepsilon]_\# = e^{-\frac{1}{\varepsilon}} p^m$, which is asymptotically close to zero in $S_\rho^m(\varepsilon)$. In the following we will use the same symbol for an element in $S_\rho^m(\varepsilon)$ and its expansion in $M_\rho^m(\varepsilon)$. As suggested by the preceding discussion, we introduce the following synthetic notation.

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

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