Space-adiabatic perturbation theory for Dirac-Bloch electrons

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Zusammenfassung

Die Arbeit untersucht im ersten Teil die durch die Dirac-Gleichung erzeugte quantenmechanische Dynamik eines Elektrons in einem kristallinen Festkörper. Dabei unterliegt das Elektron neben dem periodischen Potential des Festkörpers dem Einfluß äußerer elektrischer und magnetischer Potentiale. Man nimmt an, daß die äußeren Potentiale schwach veränderlich auf der durch das periodische Gitter festgelegten Längenskala sind und wendet die raum-adiabatische Störungstheorie an, um aufbauend auf der ungestörten Dynamik (d.h. ohne äußere Felder) die volle Dynamik für geeignete Anfangsbedingungen zu approximieren. Insbesondere erhält man, aufbauend auf den Elektronenbändern des ungestörten Problems, Unterräume des zugrundeliegenden Hilbertraumes, die bis auf Fehler beliebig hoher Ordnung im adiabatischen Parameter invariant unter der durch die Dirac-Gleichung erzeugten Zeitentwicklung sind. Der effektive Hamilton-Operator, der die quantenmechanische Dynamik innerhalb dieses Unterraums beschreibt, wird bis einschließlich der Terme erster Ordnung im adiabatischen Parameter berechnet. Weiterhin wird der semiklassiche Limes gebildet, d.h. die Dynamik innerhalb dieses Unterraums wird mit Hilfe klassicher Bewegungsgleichungen approximiert.

Im zweiten Teil der Arbeit werden dieselben Untersuchungen wie im ersten Teil für die Pauli-Gleichung durchgeführt, die sich als Grenzfall der Dirac-Gleichung ergibt, wenn man die Lichtgeschwindigkeit c gegen unendlich streben läßt. Wie im Fall der Dirac-Gleichung kann man auch für die Pauli-Gleichung entsprechende beinahe invariante Unterräume finden und den semiklassischen Limes durchführen.

Abschließend wird untersucht, wie sich die im ersten Teil auftretenden Größen in Abhängigkeit von der Lichtgeschwindigkeit c verhalten und welcher Zusammenhang zwischen ihnen und den entsprechenden Größen des zweiten Teils besteht. Insbesondere wird gezeigt, daß die Entwicklung im adiabatischen Parameter und die Entwicklung für großes c in den untersten Ordnungen kommutieren.

Abstract

In this thesis, in the first part we study the dynamics of a single electron in the periodic potential originating from a crystalline solid as governed by the Dirac equation. The electron is subject to the periodic potential of the solid and additional external electric and magnetic potentials. In many concrete situations, the external potentials are slowly varying on the scale of the periodic potential. Under this condition, we can apply the space-adiabatic perturbation theory in order to approximate the full dynamics of the problem for certain initial conditions by quantities derived from the unperturbed problem. In particular we derive, based on the electron bands of the unperturbed problem, subspaces of the underlying Hilbert space that are invariant under the time evolution of the problem up to errors of arbitrary order in the adiabatic parameter. The effective Hamiltonian that governs the dynamics inside this almost invariant subspace is computed including the first order terms in the adiabatic parameter. Furthermore we perform the semiclassical limit, i.e. we approximate the dynamics inside the subspace by classical equations of motion.

In the second part, we do the same program for the Pauli equation which is in a certain sense the limit of the Dirac equation as the speed of light c tends to infinity. As in the Dirac case, we determine subspaces that are invariant up to small errors and perform the semiclassical limit.

Finally we study how the quantities derived for the Dirac case behave as functions of c and how they are related to the quantities of the second part. In particular, we show that the expansions in the adiabatic parameter and the expansion for c large commute in lowest orders.

Contents

1 Introduction

An important problem in solid state physics is to describe the motion of electrons in a periodic crystal under the influence of external magnetic and electric fields. At temperatures considerably below the melting point of the solid, the ionic cores of the crystal have small relative displacements and can be regarded as fixed. The electrons of the solid are then subject to a fixed periodic potential generated by the cores. Neglecting the Coulomb repulsion between the electrons, one is led to a quantum mechanical one-particle problem. If the Fermi energy of the solid is small on the relativistic energy scale, as is the case for ordinary metals (see [AsMe]), the dynamics of the electrons is approximately governed by the Schrödinger equation. However, as argued in [Wi], there are materials whose periodic potential is so strong that relativistic effects cannot be neglected. In this case, one has to add relativistic corrections, such as spin-orbit coupling (see [FoWo]), to the Schrödinger Hamiltonian or to use the fully relativistic Dirac equation to describe the motion of the electrons.

In the absence of external electric and magnetic potentials, both the Schrödinger and Dirac Hamiltonian with periodic potential show a particular simple structure. Exploiting the periodicity of the problem, one obtains so-called Bloch states that are invariant under the time evolution generated by the Hamiltonian. If one probes the conduction electrons through external electromagnetic fields, the bands are not decoupled anymore. Since the external potentials that can be generated under laboratory conditions vary slowly on the scale of the periodic lattice, in the physics literature ([AsMe], [Wa], [Za]) one argues that band transitions are small and the electrons' dynamics can be described semiclassically by replacing the free kinetic energy by the band energy. Mathematically, there have been several approaches to derive a semiclassical model for electrons in a periodic potential. [MMP] and [GMMP] in a more general context use Wigner functions to derive semiclassical equations of motion in the case of vanishing external potentials. [GRT] use a wave packet ansatz to obtain on a formal level semiclassical equations for the solutions of the Schrödinger equation in the case of a constant external magnetic field and vanishing electric field. [DGR] use the same technique in a more general case including slowly varying external magnetic and electric potentials. Another approach using a wave packet ansatz can be found in [SuNi], where semiclassical equations including first order corrections are derived from the Schrödinger equation without giving a rigorous proof.

The recent approach in [PST_3] gives a rigorous derivation of semiclassical equations of motion from the quantum mechanical Schrödinger equation with slowly varying external magnetic and electric fields. The derivation of the semiclassical model is split into two parts. Using symbolic calculus, they first show on a quantum mechanical level the existence of almost invariant subspaces associated to band subspaces of the unperturbed problem and determine the time evolution inside this subspace. In a second step, they approximate the dynamics inside a single band by the flow of a classical Hamiltonian system, i.e. establish the semiclassical limit. In this thesis, we want to undertake the same program as in [PST_3] for the Dirac equation and for the Schrödinger equation with relativistic corrections. Furthermore, since the Schrödinger Hamiltonian and its relativistic corrections are approximations of the Dirac Hamiltonian, we want to study whether and in which sense the two approximations commute.

1.1 Formulation of the problem

We consider the dynamics of a single relativistic electron described by the Dirac equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \Big(m_e c^2\boldsymbol{\beta} + \hbar c(-i\nabla_x - \frac{e}{c}A(\varepsilon x))\cdot\boldsymbol{\alpha} + V_\Gamma(x) + e\phi(\varepsilon x)\Big)\,\psi(x,t) \quad (1.1)$$

with $\psi(\cdot,t)\in L^2(\mathbb{R}^3,\mathbb{C}^4)$, $t\in\mathbb{R}$. In (1.1) we use the Dirac matrices

$$\boldsymbol{\beta} = \begin{pmatrix} \mathbf{1}_{\mathbb{C}^2} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1}_{\mathbb{C}^2} \end{pmatrix} \text{ and } \boldsymbol{\alpha}_l = \begin{pmatrix} \mathbf{0} & \boldsymbol{\sigma}_l \\ \boldsymbol{\sigma}_l & \mathbf{0} \end{pmatrix}, \quad l=1,2,3$$

where $\boldsymbol{\sigma}_l$, $l=1,2,3$ are the Pauli spin matrices (see list of symbols). The potential $V_\Gamma:\mathbb{R}^3\to\mathbb{R}$ is periodic with respect to some regular lattice Γ generated through the basis $\{\gamma_1,\gamma_2,\gamma_3\}$, $\gamma_j\in\mathbb{R}^3$, i.e. $V_\Gamma(x+\gamma)=V_\Gamma(x)$ for all $x\in\mathbb{R}^3$, $\gamma\in\Gamma$ where

$$\Gamma = \{x\in\mathbb{R}^3 | x = \sum_{j=1}^{3} a_j\gamma_j, \quad a_j\in\mathbb{Z}\}.$$

The external magnetic and electric potentials $A:\mathbb{R}^3\to\mathbb{R}^3$ and $\phi:\mathbb{R}^3\to\mathbb{R}$ vary slowly on the lattice scale, as expressed through the parameter $0\le\varepsilon\ll 1$. Furthermore, in (1.1) m_e and e are the electron's mass resp. charge, $\hbar$ is the Planck constant and c the speed of light.

Assumption 1 *We assume that* V_Γ *is infinitesimally bounded with respect to* $\sqrt{1+\Delta_x}$ *and that* $\phi \in C_b^\infty(\mathbb{R}^3, \mathbb{R})$ *and* $A_j \in C_b^\infty(\mathbb{R}^3, \mathbb{R})$ *for* $j = 1, 2, 3$.

Under this assumption, the Dirac Hamiltonian

$$H^{\varepsilon,c} := m_e c^2 \boldsymbol{\beta} + \hbar c(-i\nabla_x - \frac{e}{c} A(\varepsilon x)) \cdot \boldsymbol{\alpha} + V_\Gamma(x) + e\phi(\varepsilon x) \tag{1.2}$$

is self-adjoint on $H^1(\mathbb{R}^3, \mathbb{C}^4) \subset L^2(\mathbb{R}^3, \mathbb{C}^4)$. As well-known, the solutions of (1.1) are given by $\psi(\cdot, t) = U^{\varepsilon,c}(t)\psi(\cdot, 0)$ with the unitary group

$$U^{\varepsilon,c}(t) = \exp(-iH^{\varepsilon,c}t), \quad t \in \mathbb{R} \tag{1.3}$$

which will be our object of primary interest. In this thesis, we will study the unitary group (1.3) using the facts that ε is small and c is large. To be concrete, we will determine subspaces that are, up to errors that are small if ε is small resp. c is large, invariant under the time evolution given by (1.3). Furthermore, we will determine the dynamics inside these subspaces. The type of results we are interested in (and partially also the techniques) will become clearer by giving a motivational example in the following section.

1.2 A motivational example

The following standard example of perturbation theory of operators (see [Ka], chapter VII) illustrates the goals of this thesis. Suppose $H(\kappa)$, $\kappa \in \mathbb{R}$ is a family of bounded operators on some Hilbert space $\mathcal{H}$ that is analytic in κ such that the spectrum of $H(0)$ is separated into two parts. If Λ is a circle in the complex plane enclosing one of the parts, then the corresponding spectral projector $\Pi(0)$ is given by $\Pi(0) = \int_\Lambda \mathrm{d}\zeta (H(0) - \zeta)^{-1}$. We know that for κ small enough, also $(H(\kappa) - \zeta)^{-1}$ exists for $\zeta \in \Lambda$, therefore

$$\Pi(\kappa) = \int_\Lambda \mathrm{d}\zeta (H(\kappa) - \zeta)^{-1}$$

is the spectral projector of $H(\kappa)$ on the part of the spectrum that lies inside Λ. Furthermore, we know that $\Pi(\kappa)$ is analytic in κ since the resolvent is analytic uniformly for $\zeta \in \Lambda$. The subspaces $\Pi(\kappa)\mathcal{H}$ and $(\mathbf{1} - \Pi(\kappa))\mathcal{H}$ are then invariant under the dynamics generated by $H(\kappa)$, i.e.

$$\exp(-itH(\kappa)) = \exp(-itH(\kappa)\Pi(\kappa)) \oplus \exp(-itH(\kappa)(\mathbf{1} - \Pi(\kappa))), \quad t \in \mathbb{R}.$$

However, since $\Pi(\kappa)\mathcal{H}$ and $(\mathbf{1} - \Pi(\kappa))\mathcal{H}$ depend on κ, one aims at unitarily transforming them into κ-independent reference subspaces. Using the so-called Nagy formula, one defines the unitary operator

$$U(\kappa) := (\mathbf{1} - (\Pi(\kappa) - \Pi(0)))^{-\frac{1}{2}} (\Pi(0)\Pi(\kappa) + (\mathbf{1} - \Pi(0))(\mathbf{1} - \Pi(\kappa)))$$

that is analytic in κ and maps $\Pi(\kappa)\mathcal{H}$ into $\Pi(0)\mathcal{H}$, i.e.

$$U(\kappa)\Pi(\kappa)U^*(\kappa) = \Pi(0).$$

Now, defining the effective Hamiltonian $h(\kappa) \in \mathcal{L}(\Pi(0)\mathcal{H})$ by

$$h(\kappa) \otimes \mathbf{0} := U(\kappa)H(\kappa)\Pi(\kappa)U^*(\kappa) \tag{1.4}$$

the dynamics inside $\Pi(\kappa)\mathcal{H}$ can be described with

$$\exp(itH(\kappa))\Pi(\kappa) = U^*(\kappa)\left(\exp(ith(\kappa)) \oplus \mathbf{0}\right)U(\kappa). \tag{1.5}$$

If one replaces $U(\kappa) = \sum_{l=0}^{\infty} \kappa^l U_l$, $h(\kappa) = \sum_{l=0}^{\infty} \kappa^l h_l$ and $\Pi(\kappa) = \sum_{l=0}^{\infty} \kappa^l \Pi_l$ in (1.5) by the truncated series $U^{(n)}(\kappa) = \sum_{l=0}^{n} \kappa^l U_l$ etc., the equality holds up to errors of order $\mathcal{O}(\kappa^{n+1})$.

It must be emphasized that the preceding example is meant rather to illustrate what type of results we are interested in than to explain how to obtain them. As in the example, we are in the following interested in finding (almost) invariant subspaces of a perturbed problem based on certain invariant subspaces of the corresponding unperturbed problem and to determine the dynamics therein. However there are substantial differences between the scope of this thesis and the preceding example. While in the example above and for the nonrelativistic (i.e. $c \to \infty$) limit the relevant invariant subspace of the unperturbed problem is spectral, in space-adiabatic perturbation theory (i.e. $\varepsilon \to 0$) one starts with a (in general non-spectral) band subspace of the unperturbed Hamiltonian. Clearly in the latter case the construction as given above breaks down and one has to use different techniques, in particular the symbolic calculus, to obtain similar results. Also in the nonrelativistic limit there are important differences, since the spectral subspace of the unperturbed problem corresponds to an unbounded part of the spectrum and the construction of our example cannot be used directly.

1.3 Outline

As mentioned above, we want to find subspaces that are invariant (up to "small" errors) under the unitary group $\exp(-iH^{\varepsilon,c}t)$, $t \in \mathbb{R}$, corresponding unitary transformations into a reference space and effective Hamiltonians as above in two ways, namely by expanding in the small parameters ε or $\frac{1}{c}$. The expansion in $\frac{1}{c}$ yields the Pauli Hamiltonian and its relativistic corrections as the first order terms of the effective Hamiltonian as in (1.4), using arguments similar to the standard example of the preceding section. Physically this expansion means to project onto the electronic subspace.

The expansion in ε, that yields the dynamics inside a family of bands, requires different techniques. Since there is no global spectral gap between bands, there is no spectral subspace corresponding to the band subspace of the unperturbed Hamiltonian. However, using space-adiabatic perturbation theory and the symbolic calculus (see [Teu]), we can find subspaces that are at least invariant up to errors of order $\mathcal{O}(\varepsilon^\infty)$. Again using symbolic calculus, one can also find a unitary transformation onto a reference space and an effective Hamiltonian. Clearly, the quantities obtained in these two expansions can still be expanded in terms of the other parameter respectively, therefore we will study whether resp. in which sense the two expansions commute as shown in figure 1.1.

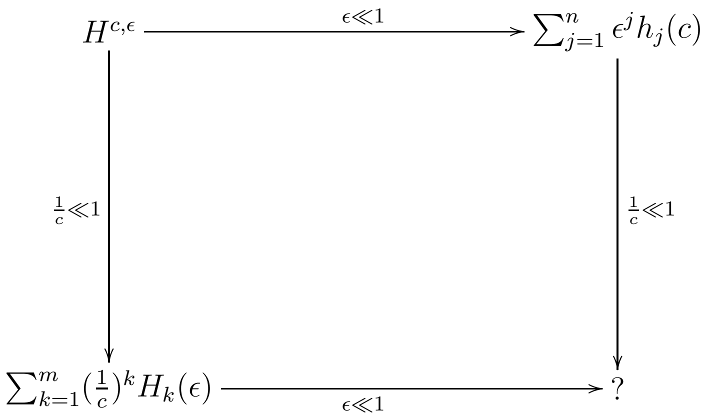

Figure 1.1: commutative diagram

In chapter 2 we apply space-adiabatic perturbation theory to the Dirac Hamiltonian $H^{\varepsilon,c}$, i.e. we study the relation between the upper left and upper right corner of the diagram. We determine subspaces that are invariant under the unitary group $\exp(-iH^{\varepsilon,c}t)$, $t \in \mathbb{R}$ up to errors of order $\mathcal{O}(\varepsilon^\infty)$, a unitary transformation into a reference space and compute the effective Hamiltonian in the lowest orders. For a single band, we derive the semiclassical limit, i.e. we approximate the dynamics of the system on the almost invariant subspace by classical equations of motion.

In chapter 3 we first study the relation between the upper left and lower left corner of the diagram, i.e. we study how the Pauli Hamiltonian $H^{\varepsilon,P}$ and its relativistic corrections approximate the Dirac Hamiltonian $H^{\varepsilon,c}$ on an appropriate subspace. Furthermore, we apply space-adiabatic perturbation theory to them, i.e. investigate the relation between the lower left and lower right corner. For the Pauli Hamiltonian, the semiclassical limit for a single band yields classical equations of motion that agree with the ones derived in [Teu] for the Schrödinger case except for two terms coming from the relativistic corrections.

In chapter 4 we investigate the relation between the upper right and lower left corner of the diagram. It turns out that the effective Hamiltonian and the related quantities derived from the Dirac Hamiltonian by applying space-adiabatic perturbation theory have norm-convergent power series expansions in $\frac{1}{c}$. Furthermore, the lowest order terms in $\frac{1}{c}$ agree with the corresponding terms derived from the Pauli Hamiltonian.

2 Dirac-Bloch electrons

In this chapter, we apply space-adiabatic perturbation theory to the Hamiltonian

$$H^\varepsilon := \boldsymbol{\beta} + (-i\nabla_x - A(\varepsilon x)) \cdot \boldsymbol{\alpha} + V_\Gamma(x) + \phi(\varepsilon x). \tag{2.1}$$

Compared to (1.2), in (2.1) we have chosen units in which the Planck constant $\hbar$, the electron mass m_e and the speed of light c are 1 and have absorbed the electron charge e into the potentials. For notational simplicity, we also dropped the superscript c.

Since we are interested in the dynamics of (2.1) we have to study the unitary group $\exp(-iH^\varepsilon t/\varepsilon), t \in \mathbb{R}$, where t/ε is used instead of t to indicate that one has to observe the time evolution over times of order ε^{-1} in order to see finite changes in the dynamics, since the external forces are of order ε. In order to recover relevant information about $\exp(-iH^\varepsilon t/\varepsilon)$ we will first identify subspaces that are invariant under the dynamics generated by the unperturbed Hamiltonian, i.e. by $H^{\varepsilon=0}$. This will be done in section 2.1 by studying the unitarily transformed Hamiltonian

$$H_Z^{\varepsilon=0} := (\mathcal{U} \otimes \mathbf{1}_{\mathbb{C}^4})\, H^{\varepsilon=0} \left(\mathcal{U}^{-1} \otimes \mathbf{1}_{\mathbb{C}^4}\right)$$

acting on $\mathcal{H}_\tau = \mathcal{U}\left(L^2(\mathbb{R}^3)\right) \otimes \mathbb{C}^4$ where $\mathcal{U}$ is the so-called Zak-transform. In the next section we will go through the usual steps of space-adiabatic perturbation theory as described in [Teu]: Given an invariant subspace of the unperturbed Hamiltonian $H_Z^{\varepsilon=0}$, we will construct a (ε-dependent) projector Π_Z^ε such that the subspace $\Pi_Z^\varepsilon \mathcal{H}_\tau$ is almost invariant under the full dynamics generated by H_Z^ε, i.e.

$$(\mathbf{1} - \Pi_Z^\varepsilon) \exp(-iH_Z^\varepsilon t/\varepsilon)\Pi_Z^\varepsilon = \mathcal{O}(\varepsilon^\infty).$$

Next, we will describe the dynamics inside $\Pi_Z^\varepsilon \mathcal{H}_\tau$ by a simpler reference Hamiltonian on a "decomposed" reference space $\mathcal{H}_r = \mathcal{K} \oplus \mathcal{K}^\perp$, i.e. we will construct a unitary mapping $U^\varepsilon : \mathcal{H}_\tau \to \mathcal{H}_r$ and a self adjoint operator $\widehat{h} \in \mathcal{L}(\mathcal{K})$ such that

$$\exp(-iH_Z^\varepsilon t/\varepsilon)\Pi_Z^\varepsilon - U^{\varepsilon *} \left(\exp(-i\widehat{h}t) \oplus \mathbf{0}_{\mathcal{K}^\perp}\right) U^\varepsilon = \mathcal{O}(\varepsilon^\infty)$$

where $\widehat{h}$ as well as U^ε are quantizations of semiclassical symbols (see appendix) which can in principle be computed to any order in ε. The result is stated in theorem 2.6 and corollary 2.8. Finally, in section 2.3 we will study the semiclassical limit of the dynamics, i.e. we will identify Hamiltonian equations in a classical phase space such that

$$\exp(iH^\varepsilon t/\varepsilon)\widehat{b}\exp(-iH^\varepsilon t/\varepsilon) - \widehat{b\circ\Phi^t}$$

is of order $\mathcal{O}(\varepsilon)$ or even of order $\mathcal{O}(\varepsilon^2)$, i.e. such that the time evolution of the Weyl-quantization of a semiclassical symbol b can be approximated up to order $\mathcal{O}(\varepsilon)$ by transporting its symbol b along the flow Φ^t of the classical system. The corresponding result is given in theorem 2.14.

Remark 2.1 *We recall the isomorphy*

$$L^2(\mathbb{R}^3,\mathcal{H}) \cong L^2(\mathbb{R}^3)\otimes\mathcal{H}$$

where $\mathcal{H}$ is any separable Hilbert space. E.g., the Hamiltonian 2.1 reads

$$\mathbf{1}_{L^2(\mathbb{R}^3)}\otimes\boldsymbol{\beta} + \sum_{l=1}^{e}(-i\partial_l - A_l(\varepsilon x))\otimes\boldsymbol{\alpha}_l + V_\Gamma(x)\otimes\mathbf{1}_{\mathbb{C}^4} + \phi(\varepsilon x)\otimes\mathbf{1}_{\mathbb{C}^4}$$

if seen as an operator on $L^2(\mathbb{R}^3)\otimes\mathbb{C}^4$. In the following we identify both notations without further notice.

2.1 The unperturbed Hamiltonian

We first recall some basic facts about the unperturbed Hamiltonian

$$H^{\varepsilon=0} = \boldsymbol{\beta} + (-i\nabla_x)\cdot\boldsymbol{\alpha} + V_\Gamma(x).$$

To formulate these results, we introduce the dual lattice Γ^* of Γ generated by the dual basis $\gamma_1^*,\gamma_2^*,\gamma_3^*$ determined by the conditions $\gamma_i\cdot\gamma_j = 2\pi\delta_{ij},\quad i,j=1,2,3.$ The centered fundamental domain M of Γ (and analogously M^* of Γ^*) is defined as

$$M = \{x\in\mathbb{R}^3 : x = \sum_{j=1}^{3} a_j\gamma_j \text{ for } a_j \in [-\frac{1}{2},\frac{1}{2}]\}.$$

In physics, M^* is called the first Brillouin zone.

2.1.1 The Zak transform

In order to bring $H^{\varepsilon=0}$ into a simpler form, we introduce (following the presentation in [Teu]) the Zak transform $\mathcal{U}\psi$ of a function $\psi \in \mathcal{S}(\mathbb{R}^3)$ by

$$(\mathcal{U}\psi)(k,y) := \sum_{\gamma\in\Gamma} e^{-i(y+\gamma)\cdot k}\psi(y+\gamma), \quad (k,y)\in\mathbb{R}^6.$$

From the definition it follows that

$$(\mathcal{U}\psi)(k,y+\gamma) = (\mathcal{U}\psi)(k,y) \quad \text{for all } \gamma\in\Gamma, \tag{2.2}$$

$$(\mathcal{U}\psi)(k+\gamma^*,y) = e^{-iy\cdot\gamma^*}(\mathcal{U}\psi)(k,y) \quad \text{for all } \gamma^*\in\Gamma^*. \tag{2.3}$$

From (2.2) one can see that for fixed $k\in\mathbb{R}^3$, $(\mathcal{U}\psi)(k,\cdot)$ is a Γ-periodic function or in other words an element of $L^2(\mathbb{T}^3)$ (provided it is square-integrable) where $\mathbb{T}^3 := \mathbb{R}^3/\Gamma$. In this context it is useful to define the Hilbert spaces

$$L^2_\tau(\mathbb{R}^3,\mathcal{H}) := \{\psi\in L^2_{loc}(\mathbb{R}^3,\mathcal{H}) : \psi(k-\gamma^*) = \tau(\gamma^*)\psi(k)\}, \tag{2.4}$$

(where $\mathcal{H}$ is any separable Hilbert space) equipped with the inner product

$$\langle\psi,\varphi\rangle = \int_{M^*} \mathrm{d}k\, \langle\psi(k),\varphi(k)\rangle_{\mathcal{H}}$$

where $\tau(\gamma^*)$ denotes multiplication with $\exp(i\gamma^*\cdot y)$. We state that with a straightforward computation $\|\mathcal{U}\psi\|_{L^2_\tau(\mathbb{R}^3,L^2(\mathbb{T}^3))} = \|\psi\|_2$ for $\psi\in\mathcal{S}(\mathbb{R}^3)$, therefore $\mathcal{U}$ extends to a norm-preserving operator from $L^2(\mathbb{R}^3)$ into $L^2_\tau(\mathbb{R}^3,L^2(\mathbb{T}^3))$.

On the other hand if we define

$$(\mathcal{U}^{-1}\varphi)(x) := \int_{M^*} \mathrm{d}k e^{ix\cdot k}\varphi(k,x)$$

for $\varphi\in C^1_\tau(\mathbb{R}^3\times\mathbb{R}^3)$ (where the subscript τ means that φ is τ-equivariant in the first and periodic in the second variable) it is also straightforward to show that $\mathcal{U}^{-1}$ extends to a norm-preserving operator from $L^2_\tau(\mathbb{R}^3,L^2(\mathbb{T}^3))$ to $L^2(\mathbb{R}^3)$. Furthermore, for $\psi\in\mathcal{S}(\mathbb{R}^3)$ we have (recall that all the sums and integrals are absolutely convergent)

$$\begin{aligned}(\mathcal{U}^{-1}\mathcal{U}\psi)(x) &= \int_{M^*}\mathrm{d}k e^{ix\cdot k}\sum_{\gamma\in\Gamma} e^{-i(x+\gamma)\cdot k}\psi(x+\gamma)\\ &= \sum_{\gamma\in\Gamma}\left(\int_{M^*}\mathrm{d}k e^{-i\gamma\cdot k}\right)\psi(x+\gamma)\\ &= \psi(x).\end{aligned}$$

By continuity we have $\mathcal{U}^{-1}\mathcal{U}\psi = \psi$ on $L^2(\mathbb{R}^3)$. To show surjectivity of $\mathcal{U}$, suppose there is a $\varphi \in L^2_\tau(\mathbb{R}^3, L^2(\mathbb{T}^3)) \setminus \mathcal{U}(L^2(\mathbb{R}^3))$. Then $\mathcal{U}\mathcal{U}^{-1}\varphi \neq \varphi$, but $\mathcal{U}^{-1}\mathcal{U}\mathcal{U}^{-1}\varphi = \mathcal{U}^{-1}\varphi$ which is a contradiction to the injectivity of $\mathcal{U}^{-1}$. Therefore $\mathcal{U}$ is unitary and $\mathcal{U}^{-1}$ is its inverse. Finally we state that $\mathcal{U} \otimes \mathbf{1}_{\mathbb{C}^4}$ is unitary from $L^2(\mathbb{R}^3, \mathbb{C}^4)$ to

$$\mathcal{H}_\tau := L^2_\tau(\mathbb{R}^3, \mathcal{H}_f) \tag{2.5}$$

with $\mathcal{H}_f := L^2(\mathbb{T}^3, \mathbb{C}^4)$.

A straightforward computation gives the Zak transforms of multiplication and differentiation operators. To simplify notation, we identify $L^2_\tau(\mathbb{R}^3, L^2(\mathbb{T}^3))$ with $L^2_\tau(\mathbb{R}^3) \otimes L^2(\mathbb{T}^3)$ (where $L^2_\tau(\mathbb{R}^3) := L^2_\tau(\mathbb{R}^3, \mathbb{C})$ is defined in the obvious way). We have

$$\mathcal{U}(-i\nabla_x)\mathcal{U}^{-1} = \mathbf{1} \otimes (-i\nabla_y) - k \otimes \mathbf{1}$$

with domain $L^2_\tau(\mathbb{R}^3) \otimes H^1(\mathbb{T}^3)$. On the other hand

$$\mathcal{U}Q\mathcal{U}^{-1} = i\nabla^\tau_k$$

on the domain $H^1_\tau(\mathbb{R}^3) \otimes L^2(\mathbb{T}^3)$ (as indicated by the superscript τ in ∇^τ_k) where Q denotes multiplication with x on the maximal domain and $H^1_\tau(\mathbb{R}^3) := H^1_{loc}(\mathbb{R}^3) \cap L^2_\tau(\mathbb{R}^3)$. For $V_\Gamma(x)$ however one has

$$\mathcal{U}V_\Gamma(x)\mathcal{U}^{-1} = \mathbf{1} \otimes V_\Gamma(y).$$

We conclude that the Zak transform of the unperturbed Hamiltonian $H^{\varepsilon=0}$ is

$$(\mathcal{U} \otimes \mathbf{1}_{\mathbb{C}^4})\, H^{\varepsilon=0} \left(\mathcal{U}^{-1} \otimes \mathbf{1}_{\mathbb{C}^4}\right) = \int^\oplus_{\mathbb{R}^3} \mathrm{d}k H_{\mathrm{per}}(k)$$

with

$$H_{\mathrm{per}}(k) = \boldsymbol{\beta} + (-i\nabla_y - k) \cdot \boldsymbol{\alpha} + V_\Gamma(y), \quad k \in \mathbb{R}^3.$$

For fixed $k \in \mathbb{R}^3$, $H_{\mathrm{per}}(k)$ is self-adjoint with domain

$$\mathcal{D} := H^1(\mathbb{T}^3, \mathbb{C}^4) \subset L^2(\mathbb{T}^3, \mathbb{C}^4) =: \mathcal{H}_f$$

independent of k. Furthermore, we know that

$$H_{\mathrm{per}}(k - \gamma^*) = \tau(\gamma^*) H_{\mathrm{per}}(k) \tau(\gamma^*)^{-1}$$

i.e. $H_{\mathrm{per}}(k)$ is τ-equivariant.

2.1.2 The spectrum of $H_{\mathbf{per}}(k)$

The structure of the spectrum of $H_{\text{per}}(k)$ is crucial for the following, therefore we consider it in detail in this subsection. First we note that the resolvent

$$R_{\text{per}}(\zeta, k) = (H_{\text{per}}(k) - \zeta)^{-1} \tag{2.6}$$

satisfies

$$\begin{aligned} R_{\text{per}}(i,k) &= R_{\text{free}}(i,k)(H_{\text{free}}(k) - i)R_{\text{per}}(i,k) \\ &= R_{\text{free}}(i,k) - R_{\text{free}}(i,k)V_\Gamma(y)R_{\text{per}}(i,k) \end{aligned} \tag{2.7}$$

with $R_{\text{free}}(\zeta, k) = (H_{\text{per}}(k) - V_\Gamma - \zeta)^{-1}$. Since $V_\Gamma(y)R_{\text{per}}(i,k)$ is bounded by assumption and $R_{\text{free}}(i,k) = (\boldsymbol{\beta}+(-i\nabla_y - k)\cdot\boldsymbol{\alpha} - i)^{-1}$ is compact (as can be shown by direct computation), we have that $R_{\text{per}}(i,k)$ is also compact and $H_{\text{per}}(k)$ has purely discrete spectrum accumulating at infinity. Since $H_{\text{per}}(k)$ is not semibounded, the labeling of eigenvalues and eigenfunctions requires additional considerations. The following lemma about the time-reversal symmetry of $H_{\text{per}}(k)$ which is also used later on enables us to prove that there is an appropriate labelling. For the lemma, we introduce the notation

$$\mathbf{S}_j := \begin{pmatrix} \boldsymbol{\sigma}_j & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\sigma}_j \end{pmatrix}, \quad j = 1, 2, 3. \tag{2.8}$$

Lemma 2.2 *$H_{per}(k)$ satisfies*

$$H_{per}(-k) = \mathcal{T}^{-1} H_{per}(k) \mathcal{T}, \quad k \in \mathbb{R}^3 \tag{2.9}$$

with $\mathcal{T}$ given by

$$\mathcal{T}\psi = S_2 \bar{\psi}, \quad \psi \in L^2(\mathbb{T}^3) \otimes \mathbb{C}^4$$

and S_2 as in 2.8. Furthermore we have

$$\langle \psi, \mathcal{T}\psi \rangle = 0 \quad \textit{for all } \psi \in L^2(\mathbb{T}^3) \otimes \mathbb{C}^4.$$

In particular, each eigenvalue of $H_{per}(0)$ is at least two-fold degenerate.

Proof. We have to compute

$$\mathcal{T}^{-1} \left(\boldsymbol{\beta} + (-i\nabla_y - k) \cdot \boldsymbol{\alpha} + V_\Gamma(y) \right) \mathcal{T}.$$

One can directly see that $\boldsymbol{\beta}$ and $V_\Gamma(y)$ commute with $\mathcal{T}$. For the remaining term $(-i\nabla_y - k)\cdot\boldsymbol{\alpha}$ we state that $\{\boldsymbol{\alpha}_3, \mathbf{S}_2\} = \{\boldsymbol{\alpha}_1, \mathbf{S}_2\} = 0$ whereas $[\boldsymbol{\alpha}_2, \mathbf{S}_2] = 0$. Together with the fact that $\boldsymbol{\alpha}_1$ and $\boldsymbol{\alpha}_3$ are real-valued whereas $\boldsymbol{\alpha}_2$ is purely imaginary it follows that

$$\mathcal{T}^{-1}\left((-i\nabla_y - k)\cdot\boldsymbol{\alpha}\right)\mathcal{T} = -\mathcal{T}^{-1}(-i\nabla_y - k)\mathcal{T}\cdot\boldsymbol{\alpha}.$$

Finally it is clear that $\mathcal{T}^{-1}(-i\nabla_y)\mathcal{T} = i\nabla_y$ and $\mathcal{T}^{-1}k\mathcal{T} = k$ and therefore (2.9) follows. The second statement becomes clear by

$$\begin{aligned}
\langle\psi, \mathcal{T}\psi\rangle &= \int_M \mathrm{d}y\, \left\langle\psi(y), S_2\bar{\psi}(y)\right\rangle_{\mathbb{C}^4} \\
&= \int_M \mathrm{d}y\, \left(\bar{\psi}_1(y)(-i\bar{\psi}_2(y)) + \bar{\psi}_2(y)(i\bar{\psi}_1(y))\right) \\
&\quad + \int_M \mathrm{d}y\, \left(\bar{\psi}_3(y)(-i\bar{\psi}_4(y)) + \bar{\psi}_4(y)(i\bar{\psi}_3(y))\right) \\
&= 0
\end{aligned}$$

■

In the special case of a inversion-symmetric potential V_Γ we have additionally the following result.

Corollary 2.3 *Let $V_\Gamma(-x) = V_\Gamma(x)$ for all $x \in \mathbb{R}^3$. Then*

$$H_{per}(k) = \mathcal{T}^{-1}\mathcal{R}^{-1}H_{per}(k)\mathcal{R}\mathcal{T}, \quad k \in \mathbb{R}^3 \tag{2.10}$$

with $\mathcal{R}$ given by

$$\mathcal{R}\psi(y) = \boldsymbol{\beta}\psi(-y), \quad \psi \in L^2(\mathbb{T}^3)\otimes\mathbb{C}^4.$$

Furthermore we have

$$\langle\psi, \mathcal{R}\mathcal{T}\psi\rangle = 0 \quad \textit{for all } \psi \in L^2(\mathbb{T}^3)\otimes\mathbb{C}^4.$$

In particular, for all $k \in \mathbb{R}^3$, each eigenvalue of $H_{per}(k)$ is at least two-fold degenerate.

Proof. We compute

$$\mathcal{R}^{-1}\left(\boldsymbol{\beta} + (-i\nabla_y - k)\cdot\boldsymbol{\alpha} + V_\Gamma(y)\right)\mathcal{R}.$$

Obviously V_Γ commutes with $\mathcal{R}$. On the other hand we have $\{\boldsymbol{\alpha}, \boldsymbol{\beta}\} = 0$ and $\mathcal{R}^{-1}(-i\nabla_y)\mathcal{R} = i\nabla_y$, therefore $\mathcal{R}^{-1}H_{\rm per}(k)\mathcal{R} = H_{\rm per}(-k)$ and (2.10) follows with lemma 2.2. Furthermore

$$
\begin{aligned}
\langle\psi, \mathcal{RT}\psi\rangle &= \int_M \mathrm{d}y\, \langle\psi(y), \boldsymbol{\beta} S_2\bar{\psi}(-y)\rangle_{\mathbb{C}^4} \\
&= \int_M \mathrm{d}y\, \big(\bar{\psi}_1(y)(-i\bar{\psi}_2(-y)) + \bar{\psi}_2(y)(i\bar{\psi}_1(-y))\big) \\
&\quad - \int_M \mathrm{d}y\, \big(\bar{\psi}_3(y)(-i\bar{\psi}_4(-y)) + \bar{\psi}_4(y)(i\bar{\psi}_3(-y))\big) \\
&= 0.
\end{aligned}
$$

■

Now we turn to labelling the eigenvalues. Clearly lemma 2.2 implies that $\sigma(H_{\rm per}(k)) = \sigma(H_{\rm per}(-k))$ and this fact enables us to label the eigenvalues of $H_{\rm per}(k)$ continuously in k such that also the symmetries of $H_{\rm per}(k)$ are reflected as stated in the following lemma.

Lemma 2.4 (Labelling of eigenvalues) *There are continuous functions $E_n : \mathbb{R}^3 \to \mathbb{R}$, $n \in \mathbb{Z}$ such that, for fixed $k \in \mathbb{R}^3$, $E_n(k), n \in \mathbb{Z}$ are the eigenvalues of $H_{per}(k)$ counted according to multiplicity in increasing order and*

$$
\begin{aligned}
E_n(k+\gamma^*) &= E_n(k) \\
E_n(-k) &= E_n(k)
\end{aligned}
$$

for $n \in \mathbb{Z}$, $k \in \mathbb{R}^3$, $\gamma^* \in \Gamma^*$.

Proof. As $H_{\rm per}(k)$ has discrete spectrum accumulating at infinity, we can clearly locally label the eigenvalues continuously. Since $\overline{M^*}$ is compact, we choose a finite cover of $\overline{M^*}$ consisting of balls $\mathcal{B}_l$, $l = -L, \dots, L$ with continuous local eigenvalue labellings $E_n^{(l)} : \mathcal{B}_l \to \mathbb{R}$, $n \in \mathbb{Z}$. We assume that this cover reflects the symmetry properties of the Hamiltonian, i.e. $\mathcal{B}_{-l} = -\mathcal{B}_l$ (including $l = 0$) and $E_n^{(-l)}(-k) = E_n^{(l)}(k)$ and for each $\mathcal{B}_l$ with $\mathcal{B}_l \cap \partial M^* \neq \emptyset$ there is $\mathcal{B}_{l'} = \mathcal{B}_l + \gamma^*$ with $E_n^{(l')}(k+\gamma^*) = E_n^{(l)}(k)$ (this is possible because $-\Gamma^* = \Gamma^*$, i.e. the reflection and the lattice symmetry commute). Now we define $E_n(k) := E_n^{(0)}(k)$ on $\mathcal{B}_0$ and turn to extend the labelling. First we recall that every continuous labelling on an interval in $\mathcal{B}_l$ is of the form $E_n = E_{n+N}^{(l)}$ for some $N \in \mathbb{Z}$. Therefore a continuous labelling on an interval in $\mathcal{B}_l \cap \mathcal{B}_{l'}$ satisfies $E_n = E_{n+N}^{(l)} = E_{n+N'}^{(l')}$ where we emphasize that $N - N' =: d(l, l')$ depends only on l, l' but not on the specific choice of the interval and that $d(l,l') = d(-l,-l')$. If we want to define $E_n(\pm k)$ for $k \in \overline{M^*}$ we just take a sequence of balls (for notational simplicity $\mathcal{B}_{\pm l}$, $l = -M,\dots,M$) such that $\pm k \in \mathcal{B}_{\pm M}$ and $\mathcal{B}_l \cap \mathcal{B}_{l+1} \cap [k,k] \neq \emptyset$ for $l = -M,\dots,M-1$ and define $E_n(\pm k) = E^{(M)}_{n+N}(k)$ where $N := \sum_{l=0}^{M-1} d(l+1,l) = \sum_{l=0}^{M-1} d(-(l+1),-l)$. One can easily show that this definition is independent of the specific choice of the sequence; obviously we have $E_n(-k) = E_n(k)$. Clearly, for $k'-k$ small we know that the sequence $\mathcal{B}_{\pm l}$, $l = -M,\dots,M$ can also be used to define $E_n(k')$. In this case $E_n(k') = E^{(M)}_{n+N}(k')$ for all k' in a neighborhood of k and therefore E_n is continuous in this neighborhood. As any continuous labelling on $\mathcal{B}_l$ is of the form $E_n = E^{(l)}_{n+N}$ we immediately have that

$$E_n(k) = E^{(l)}_{n+N(l)}(k), \quad l = -L,\dots,L, k \in \mathcal{B}_l$$

with constants $N(l)$ satisfying $N(-l) = N(l)$ as well as $N(l) - N(l') = d(l,l')$. Finally let $k \in \partial M^*$, w.l.o.g. $k \in \frac{1}{2}\gamma_1^* + span(\gamma_2^*,\gamma_3^*)$. Let $\mathcal{B}_{l_m}, m = 1,\dots,n$ be a sequence of balls such that $\frac{1}{2}\gamma_1^* \in \mathcal{B}_{l_0}$, $k \in \mathcal{B}_{l_n}$ and $\mathcal{B}_{l_m} \cap \mathcal{B}_{l_{m+1}} \cap [\frac{1}{2}\gamma_1^*, k] \neq \emptyset$ and let $\mathcal{B}_{l'_m} = \mathcal{B}_{l_m} - \gamma_1^*, m = 1,\dots,n$ be its symmetric sequence. We have $N(l_0) = N(l'_0)$ because $E_n(\frac{1}{2}\gamma_1^*) = E_n(-\frac{1}{2}\gamma_1^*)$ and $d(l_{m+1},l_m) = d(l'_{m+1},l'_m)$, hence

$$\begin{aligned} N(l_n) &= N(l_0) + \sum_{m=1}^{n} d(l_m,l_{m-1}) \\ &= N(l'_n) \end{aligned}$$

and therefore $E_n(k) = E_n(k+\gamma_1^*)$. Finally we extend E_n periodically to $\mathbb{R}^3$ and note that this extension also preserves $E_n(k) = E_n(-k)$. ■

We furthermore label the normalized eigenfunctions corresponding to $E_n(k)$ as $\varphi_n(k)$ and note that E_n as well as φ_n need not be smooth functions of k if eigenvalue crossings are present.

If the variation of V_Γ is smaller than the spectral gap c^2 of the free Hamiltonian, the periodic Hamiltonian still has a spectral gap around 0 (see [CiCh]). In this case the labeling of the eigenvalues causes no problems, and the band structure is divided into two parts. Together with the preceding considerations, we get the following schematic view on the band structure of the unperturbed Hamiltonian.

2.1.3 Regularity of the resolvent

We will also need the derivatives of the resolvent $R_{\text{per}}(\zeta,k) = (H_{\text{per}}(k)-\zeta)^{-1}$ with respect to $\zeta \in \mathbb{C}$ and $k \in \mathbb{R}^3$ in the following. Since we are going to use the symbolic calculus as presented in the appendix, we have to treat unbounded

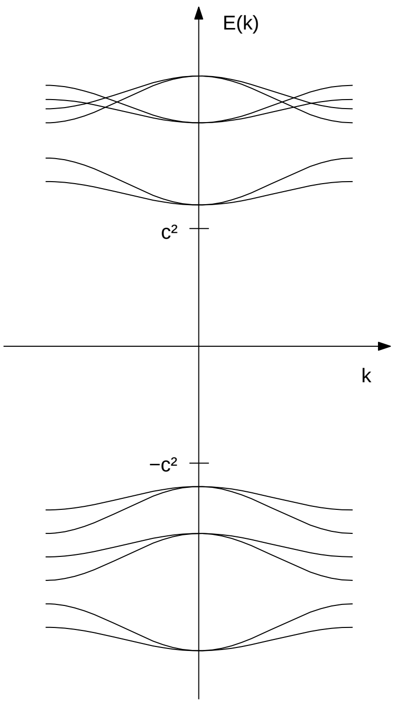

Figure 2.1: band structure of the periodic Dirac Hamiltonian

operators on $\mathcal{H}_f$ as bounded operators from $\mathcal{D}$ equipped with its own norm to $\mathcal{H}_f$. For this reason, one has to be careful about the question in which sense to take the derivatives and we will study this issue in this subsection in more detail. In this context it is useful to introduce the embedding $J : \mathcal{D} \to \mathcal{H}_f$ as $J\psi = \psi$, $\psi \in \mathcal{D}$ and we note that $\|J\|_{\mathcal{L}(\mathcal{D},\mathcal{H}_f)} \leq 1$. We start with the simple observation that $H_{\mathrm{per}}(k) - \zeta$ is invertible on the open subset $\{(k,\zeta) : \zeta \notin \sigma(H_{\mathrm{per}}(k))\} \subset \mathbb{R}^3 \times \mathbb{C}$ and that the resolvent $R_{\mathrm{per}}(\zeta, k)$ is, for each (k,ζ), a bounded operator from $\mathcal{H}_f$ to $\mathcal{D}$. From the explicit local expression for the resolvent as a von Neumann series follows that its operator norm is locally (in k,ζ) bounded. We continue with the simple equation

$$\begin{aligned} & R_{\mathrm{per}}(\zeta, k') - R_{\mathrm{per}}(\zeta, k) \\ &= R_{\mathrm{per}}(\zeta, k)\left((k - k') \cdot \boldsymbol{\alpha}\right) J R_{\mathrm{per}}(\zeta, k'). \end{aligned}$$

(which is shown as (2.7)). Together with the local boundedness of the resolvent it shows that the resolvent is continuous and differentiable with respect to k in the norm of $\mathcal{L}(\mathcal{H}_f, \mathcal{D})$, and that its partial derivatives are given by

$$\frac{\partial}{\partial k_j} R_{\mathrm{per}}(\zeta, k) = -R_{\mathrm{per}}(\zeta, k) \boldsymbol{\alpha}_j J R_{\mathrm{per}}(\zeta, k), \quad j = 1, 2, 3.$$

As well-known, the analogous argument shows that $R_{\mathrm{per}}(\zeta, k)$ is holomorphic in ζ. Inductively it follows that $R_{\mathrm{per}}(\zeta, k)$ is smooth in k and that all its derivatives are holomorphic in ζ with respect to the norm of $\mathcal{L}(\mathcal{H}_f, \mathcal{D})$. Clearly these assertions also hold true for $JR_{\mathrm{per}}(\zeta, k)$, i.e. for the resolvent seen as an operator on $\mathcal{H}_f$. Furthermore, all the derivatives are τ-equivariant.

2.2 Adiabatic perturbation theory

In this section we want to apply space-adiabatic perturbation theory in order to study the dynamics generated by the Hamiltonian (2.1). After stating our main result in theorem 2.6 we explain in detail the three steps leading to this theorem: In section 2.2.1 we construct the almost invariant subspace corresponding to an isolated family $\{E_n(k)\}_{n \in \mathcal{I}}$ (see definition 2.5). In section 2.2.2 we construct the unitary mapping to the reference space. Finally in section 2.2.3 we compute the effective Hamiltonian on the reference space.

For the unperturbed Hamiltonian H_{per}, the band subspaces given by the projectors $P_n = \int_{M^*}^{\oplus} P_n(k)$, $n \in \mathbb{N}$ where $P_n(k) = \langle \varphi_n(k), \cdot \rangle \, \varphi_n(k)$ are invariant under the dynamics generated by H_{per}, i.e.

$$[\exp(-i\mathcal{U} H_{\mathrm{per}} \mathcal{U}^{-1} t), P_n] = 0 \quad \text{for all } n \in \mathbb{N}, t \in \mathbb{R}.$$

If slowly varying external fields are present, we have to consider the Hamiltonian

$$H_Z^{\varepsilon} := \mathcal{U} H^{\varepsilon} \mathcal{U}^{-1} = \boldsymbol{\beta} + (-i\nabla_y + k - A(\varepsilon \nabla_k^{\tau})) \cdot \boldsymbol{\alpha} + V_{\Gamma}(y) + \phi(\varepsilon \nabla_k^{\tau})$$

and the band subspaces of H_{per} are in general no longer invariant, therefore we apply space-adiabatic theory to construct almost invariant subspaces. A basic requirement for applying this technique is the existence of a family of isolated bands of the unperturbed Hamiltonian.

Definition 2.5 *A family of bands $\{E_n(k)\}_{n \in \mathcal{I}}$ of eigenvalue bands of $H_{per}(k)$ with $\mathcal{I} = [I_-, I_+] \cap \mathbb{N}$ is called isolated if $\{E_n(k)\}_{n \in \mathcal{I}} \cap \{E_m(k)\}_{m \in \mathcal{I}} = \emptyset$ for all $k \in M^*$.*

Since lemma 2.2 states that each eigenvalue of $H_{\mathrm{per}}(0)$ must be at least twofold degenerate, we can exclude the case $|\mathcal{I}| = 1$, i.e. the case of a single isolated non-degenerate energy band. Furthermore we note that from the definition of an isolated band it follows that even

$$\inf_{k\in\mathbb{R}^3} dist(\bigcup_{n\in\mathcal{I}}\{E_n(k)\}, \bigcup_{m\notin\mathcal{I}}\{E_m(k)\}) > 0$$

because M^* is compact and E_n is periodic.

For the following we fix an index set $\mathcal{I}$ corresponding to an isolated family of bands. Furthermore we fix circles $\Lambda_{\mathrm{per}}(k) \subset \mathbb{C} \setminus \sigma(H_{\mathrm{per}}(k))$, $k \in \mathbb{R}^3$ such that, for each fixed k, $\Lambda_{\mathrm{per}}(k)$ is symmetric with respect to the real axis and encloses $\{E_n(k)\}_{n\in\mathcal{I}}$. We also assume that $\Lambda_{\mathrm{per}}(k+\gamma^*) = \Lambda_{\mathrm{per}}(k)$ as well as $\Lambda_{\mathrm{per}}(-k) = \Lambda_{\mathrm{per}}(k)$ for all $\gamma^* \in \Gamma^*$ and that the radius of $\Lambda_{\mathrm{per}}(k)$ is bounded. W.l.o.g. we choose $\Lambda_{\mathrm{per}}(k)$ piecewise constant in k and assume that there is an open set $O_{\mathrm{per}} \subset \mathbb{C}\times\mathbb{R}^3$ and a closed set $K_{\mathrm{per}} \subset \mathbb{C}\times\mathbb{R}^3$ with $K_{\mathrm{per}} \cap \mathbb{C}\times\bar{\mathcal{B}}(r,0)$ compact for any r such that

$$\bigcup_{k\in\mathbb{R}^3} (\Lambda_{\mathrm{per}}(k)\times\{k\}) \subset K_{\mathrm{per}} \subset O_{\mathrm{per}} \subset \bigcup_{k\in\mathbb{R}^3} (\mathbb{C}\setminus\sigma(H_{\mathrm{per}}(k))\times\{k\}) \tag{2.11}$$

For simplicity we also assume that O_{per} and K_{per} are periodic in k, i.e. $O_{\mathrm{per}} + (\gamma^*, 0) = O_{\mathrm{per}}$ for $\gamma^* \in \Gamma^*$ etc. If we introduce the spectral projector

$$\begin{aligned} P_{\mathrm{per}}(k) \quad &:= \int_{\Lambda_{\mathrm{per}}(k)} \mathrm{d}\zeta R_{\mathrm{per}}(\zeta,k) \\ &= \sum_{n\in\mathcal{I}} \langle\varphi_n(k),\cdot\rangle\,\varphi_n(k) \end{aligned}$$

corresponding to the family $\{E_n(k)\}_{k\in\mathcal{I}}$, it follows immediately by the gap condition that $P_{\mathrm{per}}(k)$ is smooth in k although, due to eigenvalue crossings, we cannot assure that the φ_n itselves are smooth functions of k. However, it is shown in [Pa] that there is a smooth isometry-valued map $U_{\mathrm{per}}: \mathbb{R}^3 \to \mathcal{U}(\mathcal{H}_f)$ such that

$$U_{\mathrm{per}}(k)^* P_{\mathrm{per}}(k) U_{\mathrm{per}}(k) = P_{\mathrm{per}}(0) =: \pi_r$$

and such that U_{per} is right-τ-equivariant, i.e.

$$U_{\mathrm{per}}(k+\gamma^*) = U_{\mathrm{per}}(k)\tau(\gamma^*).$$

If we choose $\chi_n := \varphi_n(0)$, $n = 1,\dots,l$ as a basis of $\mathrm{Ran}P_{\mathrm{per}}(0) =: \mathcal{K}_f \cong \mathbb{C}^N$ with $N = |\mathcal{I}|$, then

$$\psi_n(k) := U_{\mathrm{per}}(k)\chi_n$$

are smooth τ-equivariant functions, i.e. $\psi_n(k-\gamma^*) = \tau(\gamma^*)\psi_n(k)$, such that $P_{\rm per}(k) = \sum_{n\in\mathcal{I}} \langle \psi_n(k), \cdot\rangle\, \psi_n(k)$, a fact that will be essentially for the construction of the unitary u_0 in section 2.2.2. Note that in general $\psi_n(k)$ need not be eigenfunctions of $H_{\rm per}(k)$ any more. To formulate our main theorem, we introduce the reference Hilbert space

$$\mathcal{H}_r := L^2_{\tau=\mathbf{1}}(\mathbb{R}^3, \mathcal{H}_f) \tag{2.12}$$

and the orthogonal decomposition $\mathcal{H}_f = \mathcal{K}_f \oplus \mathcal{K}_f^\perp$. $\mathcal{K}_f$ is understood to be equipped with the basis χ_ν, $\nu = 1,\ldots,N$. An operator A in $\mathcal{L}(\mathcal{K}_f)$ can therefore be identified with the matrix given $\Big(\langle \chi_\nu, A\chi_m\rangle_{\mathcal{H}_f}\Big)_{\nu,\mu=1,\ldots,N}$, which we will do implicitly in the following. We furthermore have

$$\mathcal{H}_r \cong L^2_{\tau=\mathbf{1}}(\mathbb{R}^3, \mathcal{K}_f) \oplus L^2_{\tau=\mathbf{1}}(\mathbb{R}^3, \mathcal{K}_f^\perp) =: \mathcal{K} \oplus \mathcal{K}^\perp \tag{2.13}$$

and for symbols $a \in S^{\mathbf{1}}_{\tau\equiv\mathbf{1}}(\varepsilon, \mathcal{L}(\mathcal{K}_f))$ and $b \in S^{\mathbf{1}}_{\tau\equiv\mathbf{1}}(\varepsilon, \mathcal{L}(\mathcal{K}_f^\perp))$ we obviously have that $a \oplus b \in S^{\mathbf{1}}_{\tau\equiv\mathbf{1}}(\varepsilon, \mathcal{L}(\mathcal{H}_f))$ and $\widehat{a\oplus b} = \widehat{a} \oplus \widehat{b}$. We recall the definitions and results about Weyl quantization for τ-equivariant symbols as given in the appendix and state our main theorem.

Theorem 2.6 (Peierls substitution) *Let $\{E_n\}_{n\in\mathcal{I}}$ be an isolated family of bands in the sense of Definition 2.5 and let Assumption (A1) be satisfied. Then there exist*

(i) an orthogonal projection $\Pi^\varepsilon_Z \in \mathcal{L}(\mathcal{H}_\tau)$,

(ii) a unitary map $U^\varepsilon_Z \in \mathcal{L}(\mathcal{H}_\tau, \mathcal{H}_r)$, and

(iii) a self-adjoint operator $\widehat{\mathbf{h}} \in L^2_{\tau=\mathbf{1}}(\mathbb{R}^3, \mathcal{K}_f)$

such that

$$\|[\exp(-iH^\varepsilon_Z t), \Pi^\varepsilon_Z]\| = \mathcal{O}(\varepsilon^\infty(1+|t|))$$

and

$$\left\|\exp(-it\widehat{H}t)\Pi^\varepsilon_Z - U^{\varepsilon *}\Big(\exp(-i\widehat{\mathbf{h}}t) \oplus \mathbf{0}_{\mathcal{K}^\perp}\Big)U^\varepsilon\right\| = \mathcal{O}(\varepsilon^\infty(1+|t|)). \tag{2.14}$$

The effective Hamiltonian $\widehat{\mathbf{h}}$ is the Weyl quantization of a semiclassical symbol $\mathbf{h} \in S^1_{\tau\equiv\mathbf{1}}(\varepsilon, \mathcal{L}(\mathcal{K}_f))$ whose asymptotic expansion in ε can be computed to any order. Its principal symbol is given by the matrix elements

$$(\mathbf{h}_0)_{\nu,\mu}(q,p) = \big\langle \psi_\nu(q - A(p)), H_0(q,p)\psi_\mu(q-A(p))\big\rangle\,, \quad \nu,\mu \in \{1,\ldots,N\}$$

where H_0 is defined in (2.16).

Remark 2.7 *We use the boldface letter* $\mathbf{h}$ *for the symbol of the effective Hamiltonian in order to emphasize that* $\mathbf{h}$ *is matrix-valued and to be consistent with section 2.3, in particular with the notation introduced in (2.34) and (2.35).*

If the family of bands consists of a single eigenvalue (which is in particular the case if $N = 2$ and V_Γ is inversion-symmetric), also the subprincipal symbol of $\mathbf{h}$ can be computed easily.

Corollary 2.8 *Let the family* $\{E_n\}_{n\in\mathcal{I}}$ *consist of a single* N*-fold degenerate eigenvalue* $E_*(k)$*. Then we have (in the notation of theorem 2.6)*

$$\mathbf{h}_0(q,p) = (E_*(\widetilde{q}) + \phi(p))\,\mathbf{1}_{\mathcal{K}_f}$$

and

$$(\mathbf{h}_1)_{\nu,\mu}(q,p) = -F_{Lor}(\widetilde{q},p)\cdot\mathcal{A}_{\nu,\mu}(\widetilde{q}) - B(p)\cdot\mathcal{M}_{\nu,\mu}(\widetilde{q}), \tag{2.15}$$

where $\widetilde{q} = q - A(p)$*,* $\nu,\mu = 1,\dots,N$*.* F_{Lor}*,* $\mathcal{A}$ *and* $\mathcal{M}$ *are defined by*

$$F_{Lor}(k,p) := -\nabla\phi(p) + \nabla E_*(k)\times B(p),$$

$$\mathcal{A}_{\nu,\mu}(k) := i\,\langle\psi_\nu(k), \nabla_k\psi_\mu(k)\rangle_{\mathcal{H}_f}$$

and

$$\mathcal{M}_{\nu,\mu}(k) := \frac{i}{2}\,\langle\nabla_k\psi_\nu(k), \times(H_{per}(k) - E_*(k))\nabla_k\psi_\mu(k)\rangle_{\mathcal{H}_f}\,.$$

Theorem 2.6 is a consequence of the following propositions 2.9, 2.12 and the proof at the end of subsection 2.2.3. The proof of corollary 2.8 is also given in subsection 2.2.3.

To start, we state that H^ε_Z is obviously the (restriction of the) Weyl quantization of the τ-equivariant symbol $H_0 \in S^w_\tau(\varepsilon, \mathcal{L}(\mathcal{D},\mathcal{H}_f))$ given by

$$\begin{aligned} H_0(q,p) &= \boldsymbol{\beta} + (-i\nabla_y + q - A(p))\cdot\boldsymbol{\alpha} + V_\Gamma(y) + \phi(p) \\ &= H_{\mathrm{per}}(q - A(p)) + \phi(p) \end{aligned} \tag{2.16}$$

with $w(q,p) := \sqrt{1+q^2}$. We also note that all the theorems are valid for any Hamiltonian which is the quantization of a semiclassical symbol H with principal value H_0. The following proofs follow the presentation in [Teu].

2.2.1 The almost invariant subspace

In this section we construct the almost invariant subspace.

Proposition 2.9 *Let $\{E_n\}_{n\in\mathcal{I}}$ be an isolated family of bands and let Assumption (A1) be satisfied. Then there exists an orthogonal projection $\Pi^\varepsilon_Z \in \mathcal{L}(\mathcal{H}_\tau)$ such that*

$$\|[\exp(-iH^\varepsilon_Z t), \Pi^\varepsilon_Z]\| = \mathcal{O}(\varepsilon^\infty(1+|t|))$$

and $\|\Pi^\varepsilon_Z - \widehat{\pi}\|_{\mathcal{L}(\mathcal{H}_f)} = \mathcal{O}(\varepsilon^\infty)$, where $\widehat{\pi} \in \mathcal{L}(\mathcal{H}_\tau)$ is the Weyl quantization of a τ-equivariant semiclassical symbol

$$\pi \asymp \sum_{j\geq 0} \varepsilon^j \pi_j \quad \textit{in } S^{\mathbf{1}}_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_f)),$$

with $\pi_0(q,p) = P_{per}(q - A(p))$.

We first construct the formal power series $\sum_{j\geq 0}\varepsilon^j\pi_j$. Since formally the symbol H takes values in $\mathcal{L}(\mathcal{D},\mathcal{H}_f)$ where $\mathcal{D}$ and $\mathcal{H}_f$ are seen as different Hilbert spaces, it is helpful to use the continuous injection $J:\mathcal{D}\to\mathcal{H}_f$ as defined in section 2.1.3 in the following lemma in order to distinguish between symbols taking values in $\mathcal{L}(\mathcal{H}_f,\mathcal{D})$ and their extension to symbols with values in $\mathcal{L}(\mathcal{H}_f)$. In the statement of proposition 2.9 however, we can drop the lenghty notation as explained in the proof.

Lemma 2.10 *Let $w(q,p) = \sqrt{1+q^2}$. Then there is a unique formal power series of symbols*

$$\pi = \sum_{j\geq 0} \varepsilon^j \pi_j \quad \textit{in } M^w_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_f,\mathcal{D})),$$

whose principal symbol π_0 satisfies $\pi_0(q,p) = P_{per}(q - A(p))$ such that

(i) $J\pi\sharp J\pi = J\pi$,

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

(iii) $H\sharp\pi = (H\sharp\pi)^*$.

Proof. First we want to prove the uniqueness of a π with the desired properties. Obviously $\pi_0(q,p) = P_{\rm per}(q-A(p))$ is the only symbol satisfying (i)-(iii) up to order $\mathcal{O}(\varepsilon)$. Now we proceed by induction and suppose we have found $\pi^{(n)} = \sum_{j=0}^n \varepsilon^j\pi_j$ satisfying (i)-(iii) up to order $\mathcal{O}(\varepsilon^{n+1})$, in particular with

$$\pi^{(n)}\sharp\pi^{(n)} - \pi^{(n)} =: \varepsilon^{n+1}G_{n+1} + \mathcal{O}(\varepsilon^{n+2}).$$

Then π_{n+1} must satisfy

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

Now, since

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

and vice versa, it follows that the diagonal part of π_{n+1}

$$\pi^D_{n+1} := \pi_0\pi_{n+1}\pi_0 + (\mathbf{1}-\pi_0)\pi_{n+1}(\mathbf{1}-\pi_0)$$

has to be G_{n+1} whereas we don't have any constraint on the off-diagonal part. It remains now to show that $\pi_0\pi_{n+1}(\mathbf{1}-\pi_0)$ is uniquely determined by (iii) since $(\mathbf{1}-\pi_0)\pi_{n+1}\pi_0$ then follows with (ii). To this end, with $\omega^{(n)} := \pi^{(n)} + \varepsilon^{n+1}G_{n+1}$ we define

$$[H,\omega^{(n)}]_\sharp =: \varepsilon^{n+1}F_{n+1} + \mathcal{O}(\varepsilon^{n+2})$$

and conclude that the off-diagonal part of π_{n+1}, i.e.

$$\pi^{OD}_{n+1} = \pi_0\pi_{n+1}(\mathbf{1}-\pi_0) + (\mathbf{1}-\pi_0)\pi_{n+1}\pi_0$$

must satisfy

$$[H_0,\pi^{OD}_{n+1}] = -F_{n+1}.$$

In particular, one has

$$H_0\pi_0\pi_{n+1}(\mathbf{1}-\pi_0) - \pi_0\pi_{n+1}(\mathbf{1}-\pi_0)H_0 = -\pi_0F_{n+1}(\mathbf{1}-\pi_0)$$

determining $\pi^{OD1}_{n+1} := \pi_0\pi_{n+1}(\mathbf{1}-\pi_0)$. Now if there were two solutions, then there must be a π^{OD1}_{n+1} satisfying

$$\begin{aligned}&[H_0,\pi^{OD1}_{n+1}] = 0\\ \iff\quad &[H_0 - E,\pi^{OD1}_{n+1}] = 0\\ \iff\quad &\pi^{OD1}_{n+1} = (H_0-E)\,\pi_0\pi^{OD1}_{n+1}(\mathbf{1}-\pi_0)\,(H_0-E)^{-1}\end{aligned}$$

with any scalar-valued symbol E such that $H_0 - E$ is invertible on $(\mathbf{1}-\pi_0)\,\mathcal{H}_f$. If $E_1(k)$ and $E_N(k)$ are the lowest resp. highest energy band in our isolated family, then we choose $E(q,p) := \frac{1}{2}(E_N(q-A(p)) + E_1(q-A(p)))$. It follows for fixed $z \in \mathbb{R}^6$ that

$$\begin{aligned} &\left\|\pi_{n+1}^{OD1}(z)\right\| \\ &\leq \ \left\|(H_0(z)-E(z))\,\pi_0(z)\right\| \left\|\pi_{n+1}^{OD1}(z)\right\| \left\|(\mathbf{1}-\pi_0(z))\,(H_0(z)-E(z))^{-1}\right\| \\ &= \ : C\left\|\pi_{n+1}^{OD1}(z)\right\|. \end{aligned}$$

Now by construction it follows that

$$\left\|(H_0(z)-E(z))\,\pi_0(z)\right\| = \frac{1}{2}(E_N(q-A(p)) - E_1(q-A(p)))$$

whereas

$$\left\|(\mathbf{1}-\pi_0(z))\,(H_0(z)-E(z))^{-1}\right\| < \left(\frac{1}{2}(E_N(q-A(p)) - E_1(q-A(p)))\right)^{-1}$$

by the gap condition, i.e. $C<1$ and $\pi_{n+1}^{OD1}(z) = 0$.

Now we turn to the construction of π. To this end, let $\Lambda_{\mathrm{per}}(k)$ be the circles enclosing $\{E_n(k)\}_{n\in\mathcal{I}}$ as defined at the beginning of section 2.2.

First we construct a Moyal resolvent for the symbol $H-\zeta$, $\zeta\in\mathbb{C}$, i.e. a formal power series $R(\zeta)$ with coefficients $R_j(\zeta) \in C^\infty(O_\zeta, \mathcal{L}(\mathcal{H}_f,\mathcal{D}))$ where $O_\zeta := \{(q,p)\in\mathbb{R}^6 : (\zeta-\phi(p), q-A(p)) \in O_{\mathrm{per}}\}$such that

$$(H-\zeta)\sharp\sum_{j\geq 0}\varepsilon^j R_j(\zeta) = \mathbf{1}_{\mathcal{H}_f} \text{ and } \sum_{j\geq 0}\varepsilon^j R_j(\zeta)\sharp(H-\zeta) = \mathbf{1}_{\mathcal{D}} \tag{2.17}$$

for all $z\in O_\zeta$. Note that although $\sum_{j\geq 0}\varepsilon^j R_j(\zeta)$ is in a strict sense not a formal power series of symbols as it is not defined on the whole $\mathbb{R}^6$ but just on the open subset O_ζ, the Weyl product as a local operation is well-defined. If one regards the following expressions and equalities as functions of both z and ζ, they are understood as defined (resp. as valid) on the open subset $O := \{(\zeta,q,p) : (\zeta-\phi(p), q-A(p)) \in O_{\mathrm{per}}\} \subset \mathbb{C}\times\mathbb{R}^6$.

Clearly we must have

$$R_0(\zeta) = (H_0-\zeta)^{-1} \quad \text{on } O_\zeta$$

with $R_0(\zeta)\in\mathcal{L}(\mathcal{H}_f,\mathcal{D})$ on O_ζ. Since $R_0(\zeta,q,p) = R_{\mathrm{per}}(\zeta-\phi(p), q-A(p))$, it follows from section 2.1.3 that $R_0(\zeta)$ is smooth and furthermore that its derivatives are in $\mathcal{L}(\mathcal{H}_f,\mathcal{D})$ and depend holomorphically on ζ. Now we can construct $R_j(\zeta)$, $j\geq 1$

inductively: Suppose $R^{(n)}(\zeta) = \sum_{j\le n} \varepsilon^j R_j(\zeta)$ satisfies the first equation in (2.17) up to order $\mathcal{O}(\varepsilon^{n+1})$, i.e.

$$(H-\zeta)\sharp R^{(n)}(\zeta) = \mathbf{1}_{\mathcal{H}_f} + \varepsilon^{n+1} E_{n+1}(\zeta) + \mathcal{O}(\varepsilon^{n+2}) \tag{2.18}$$

with $E_{n+1}(\zeta) \in C^\infty(O_\zeta, \mathcal{L}(\mathcal{H}_f))$. If we choose

$$R_{n+1}(\zeta) := -R_0(\zeta) E_{n+1}(\zeta)$$

we have immediately that $R_{n+1}(\zeta) \in C^\infty(O_\zeta, \mathcal{L}(\mathcal{H}_f, \mathcal{D}))$ and that $R^{(n+1)}(\zeta) := R^{(n)}(\zeta) + \varepsilon^{n+1} R_{n+1}(\zeta)$ satisfies the first equality in (2.17) up to order $\mathcal{O}(\varepsilon^{n+2})$. In an analogous way one can construct a formal power series $\widetilde{R}$ which satisfies the second equality in (2.17). Using the associativity of the Moyal product we have

$$\widetilde{R}(\zeta) = \widetilde{R}(\zeta)\sharp(H-\zeta)\sharp R(\zeta) = R(\zeta) \quad \text{for } (\zeta, z) \in O,$$

i.e. both symbols agree. From (2.17) it also follows that R satisfies the resolvent equation

$$R(\zeta) - R(\zeta') = (\zeta - \zeta')\, R(\zeta)\sharp J R(\zeta') \quad \text{for } (\zeta, z) \in O.$$

Furthermore we have for all $\varphi \in \mathcal{H}_f$, $\psi \in \mathcal{D}$

$$\begin{aligned}&\left\langle \varphi, (JR(\zeta))^*\sharp(H-\bar\zeta)\psi \right\rangle_{\mathcal{H}_f} \\ &= \ \langle (H-\zeta)\sharp R(\zeta)\varphi, \psi\rangle_{\mathcal{H}_f} = \langle \varphi, \psi\rangle_{\mathcal{H}_f},\end{aligned}$$

i.e. $(JR(\zeta))^* \sharp (H-\bar\zeta) = J$. Moyal-multiplying from right with $R(\bar\zeta)$ leads to

$$(JR(\zeta))^* = JR(\bar\zeta) \quad \text{for } (\zeta, z) \in O.$$

Next we define the formal power series π through

$$\pi_j(z) := \frac{i}{2\pi} \int_{\Lambda(z)} \mathrm{d}\zeta R_j(\zeta)(z), \quad z = (q,p) \in \mathbb{R}^6$$

with $\Lambda(z) := \Lambda_{\mathrm{per}}(q - A(p)) + \phi(p)$ for $z = (q,p) \in \mathbb{R}^6$. Obviously, π_j is well-defined and takes values in $\mathcal{L}(\mathcal{H}_f, \mathcal{D})$. Furthermore we know that $R_j(\zeta)$ and its derivatives with respect to z depend holomorphically on ζ, therefore

$$\pi_j(z) = \frac{i}{2\pi} \int_{\Lambda(z_0)} \mathrm{d}\zeta R_j(\zeta)(z), \quad z \in \mathcal{U}(z_0)$$

for a neighborhood $\mathcal{U}(z_0)$ of z_0. Since Λ_{z_0} is compact, π_j is smooth with

$$\partial^\alpha \pi_j(z) = \frac{i}{2\pi} \int_{\Lambda(z)} \mathrm{d}\zeta \partial_z^\alpha R_j(\zeta)(z), \quad z \in \mathbb{R}^6, \alpha \in \mathbb{N}^3 \tag{2.19}$$

where we changed the domain of integration back to $\Lambda(z)$. Now we can interchange integration and Moyal-multiplying to get

$$\begin{aligned}(J\pi \sharp J\pi) &= \left(\frac{i}{2\pi}\right)^2 \int_\Lambda \mathrm{d}\zeta \int_{\Lambda'} \mathrm{d}\zeta' JR(\zeta) \sharp JR(\zeta') \\ &= \left(\frac{i}{2\pi}\right)^2 \int_\Lambda \mathrm{d}\zeta \int_{\Lambda'} \mathrm{d}\zeta' J\left(R(\zeta) - R(\zeta')\right)(\zeta - \zeta')^{-1} \\ &= \frac{i}{2\pi} \int_\Lambda \mathrm{d}\zeta JR(\zeta) = J\pi,\end{aligned}$$

where Λ stands for $\Lambda(z)$ and $\Lambda' = \Lambda'(z)$ is a slightly larger circle. Furthermore we have $(J\pi)^* = (J\pi)$ due to $(JR(\zeta))^* = (JR(\bar{\zeta}))$ and symmetry of $\Lambda(z)$ with respect to the real axis. For the same reason we have

$$\begin{aligned}(H \sharp \pi)^* &= \frac{i}{2\pi} \int_\Lambda \mathrm{d}\bar{\zeta}\,(H \sharp R(\zeta))^* \\ &= \frac{i}{2\pi} \int_\Lambda \mathrm{d}\bar{\zeta}\left(\mathbf{1}_{\mathcal{H}_f} + \zeta JR(\zeta)\right)^* \\ &= \frac{i}{2\pi} \int_\Lambda \mathrm{d}\bar{\zeta}\left(\mathbf{1}_{\mathcal{H}_f} + \bar{\zeta} JR(\bar{\zeta})\right) \\ &= \frac{i}{2\pi} \int_\Lambda \mathrm{d}\zeta H \sharp R(\zeta) \\ &= H \sharp \pi.\end{aligned}$$

We are left to show that $\pi \in M_\tau^w(\varepsilon, \mathcal{L}(\mathcal{H}_f, \mathcal{D}))$. The τ-equivariance of π_j follows directly from the fact that $R(\zeta)$ is τ-equivariant and from the Γ^*-periodicity of Λ. Furthermore for all $j \in \mathbb{N}$, $\alpha \in \mathbb{N}^3$ and $z \in \mathbb{R}^6$ we have

$$\|\partial^\alpha \pi_j(z)\|_{\mathcal{L}(\mathcal{H}_f, \mathcal{D})} \leq 2\pi C_r \sup_{\zeta \in \Lambda_z} \|\partial_z^\alpha R_j(\zeta, z)\|_{\mathcal{L}(\mathcal{H}_f, \mathcal{D})}. \tag{2.20}$$

We turn to estimate the right hand side by induction w.r.t. $j \in \mathbb{N}$. Using the τ-equivariance of $\partial_z^\alpha R_0(\zeta)$ we have (for $z = (q, p)$ and $[z] := (q - \gamma^*, p)$ such that

$\gamma^* \in \Gamma^*, q - \gamma^* \in M^*)$

$$\begin{aligned}
&\sup_{\zeta\in\Lambda(z)} \|\partial_z^\alpha R_0(\zeta,z)\|_{\mathcal{L}(\mathcal{H}_f,\mathcal{D})} \\
&\quad = \sup_{\zeta\in\Lambda([z])} \left\|\tau(\gamma^*)\partial_z^\alpha R_0(\zeta,[z])\tau^{-1}(\gamma^*)\right\|_{\mathcal{L}(\mathcal{H}_f,\mathcal{D})} \\
&\quad \le \sup_{\zeta\in\Lambda([z])} \|\tau(\gamma^*)\|_{\mathcal{L}(\mathcal{D})} \|\partial_z^\alpha R_0(\zeta,[z])\|_{\mathcal{L}(\mathcal{H}_f,\mathcal{D})} \left\|\tau^{-1}(\gamma^*)\right\|_{\mathcal{L}(\mathcal{H}_f)} \\
&\quad \le \sup_{\zeta\in\Lambda([z])} w(\gamma^*,p) \|\partial_z^\alpha R_0(\zeta,[z])\|_{\mathcal{L}(\mathcal{H}_f,\mathcal{D})} \\
&\quad \le \sqrt{2}w(z) \sup_{z\in M^*\times\mathbb{R}^3} \sup_{\zeta\in\Lambda(z)} \|\partial_z^\alpha R_0(\zeta,z)\|_{\mathcal{L}(\mathcal{H}_f,\mathcal{D})} .
\end{aligned}$$

Here we used that $w(x) \le \sqrt{2}w(y-x)w(y)$ for $x, y \in \mathbb{R}^6$ and that $\tau(\gamma^*)$ is unitary as well as $\|\tau(\gamma^*)\|_{\mathcal{L}(\mathcal{D})} \le \langle\gamma^*\rangle$ as follows by direct computation. Using that $R_0(\zeta, z)$ is the composition of the functions $(\zeta, q, p) \mapsto (\zeta - \phi(p), q - A(p))$ and $(\zeta, k) \mapsto (H_{\rm per}(k) - \zeta)^{-1}$ we have furthermore

$$\begin{aligned}
&\sup_{z\in M^*\times\mathbb{R}^3} \sup_{\zeta\in\Lambda(z)} \|\partial_z^\alpha R_0(\zeta,(q,p))\|_{\mathcal{L}(\mathcal{H}_f)} \\
&\le C \max_{|\beta|\le|\alpha|} \max_{n\le|\alpha|} \sup_{k\in M^*+\mathcal{B}(\|A\|_\infty)} \sup_{\zeta\in\Lambda_{\rm per}(k)} \left\|\partial_k^\beta \partial_\zeta^n \left(H_{\rm per}(k)-\zeta\right)^{-1}\right\|_{\mathcal{L}(\mathcal{H}_f,\mathcal{D})} \\
&\quad \times \max_{|\beta|\le|\alpha|} \left\|\partial_p^\beta A\right\|_\infty \max_{|\beta|\le|\alpha|} \left\|\partial_p^\beta \phi\right\|_\infty
\end{aligned}$$

where C is some constant and, as usual, $\mathcal{B}(r)$ denotes a unit ball of radius r around the origin and $\|f\|_\infty := \sup_{x\in\mathbb{R}^3} |f(x)|$ for any function $f : \mathbb{R}^3 \to \mathbb{R}$. It follows that

$$\sup_{z\in\mathbb{R}^6} \sup_{\zeta\in\Lambda(z)} w^{-1}(z) \|\partial_z^\alpha R_j(\zeta,z)\|_{\mathcal{L}(\mathcal{H}_f,\mathcal{D})} < \infty \quad \text{for all } \alpha \in \mathbb{N}^3 \tag{2.21}$$

for $j = 0$. We proceed by induction and assume that (2.21) holds for $j \le n$. Then E_{n+1} as defined in 2.18 satisfies

$$\sup_{z\in\mathbb{R}^6} \sup_{\zeta\in\Lambda(z)} w^{-2}(z) \|\partial_z^\alpha E(\zeta,z)\|_{\mathcal{L}(\mathcal{H}_f)} < \infty \quad \text{for all } \alpha \in \mathbb{N}^3$$

by induction hypothesis and because of $H \in S^w_\tau(\varepsilon, \mathcal{L}(\mathcal{D}, \mathcal{H}_f))$. On the other hand E_{n+1} is τ-equivariant and τ is unitary, therefore $\|\partial_z^\alpha E(\zeta,z)\|_{\mathcal{L}(\mathcal{H}_f)}$ is periodic in q and we even have

$$\sup_{z\in\mathbb{R}^6} \sup_{\zeta\in\Lambda(z)} \|\partial_z^\alpha E(\zeta,z)\|_{\mathcal{L}(\mathcal{H}_f)} < \infty \quad \text{for all } \alpha \in \mathbb{N}^3.$$

Now (2.21) follows immediately for $R_{n+1} = -R_0 E_{n+1}$. We conclude from (2.20) that $\pi \in M^w_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_f, \mathcal{D}))$. ■

Remark 2.11 *For bounded self-adjoint symbols H and π we would have*

$$H\sharp\pi - (H\sharp\pi)^* = H\sharp\pi - \pi\sharp H$$

i.e. the expression $H\sharp\pi - (H\sharp\pi)^*$ in lemma 2.10 would be just the Moyal-commutator of H and π. However,in our case, the first expression is easier to handle since formally $\pi\sharp H$ is in our case a symbol taking values in $\mathcal{L}(\mathcal{D})$ but not in $\mathcal{L}(\mathcal{H}_f)$. For the following consideration, our expression will serve us as well.

Proof. (of proposition 2.9) From the projector $\pi \in M^w_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_f, \mathcal{D}))$ constructed in the previous lemma one obtains by resummation a semiclassical symbol in $S^w_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_f, \mathcal{D}))$ which we also denote by π, i.e.

$$\pi \asymp \sum_{j\geq 0} \varepsilon^j \pi_j \quad \text{in } S^w_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_f, \mathcal{D})).$$

From the definition and using τ-equivariance, it follows that

$$J\pi \asymp \sum_{j\geq 0} \varepsilon^j J\pi_j \quad \text{in } S^{\mathbf{1}}_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_f)).$$

The quantization of π resp. $J\pi$ requires some care. Clearly, the quantization $\mathcal{W}(J\pi) : \mathcal{S}'(\mathbb{R}^3, \mathcal{H}_f) \to \mathcal{S}'(\mathbb{R}^3, \mathcal{H}_f)$ of $J\pi$ restricts to a bounded operator $\widehat{J\pi} \in \mathcal{L}(\mathcal{H}_\tau)$ which satisfies

$$\left(\widehat{J\pi}\right)^2 - J\pi = \mathcal{O}(\varepsilon^\infty) \text{ and } \widehat{J\pi}^* = \widehat{J\pi} \tag{2.22}$$

as follows from lemma 2.10. Next, we want to show that $\mathcal{W}(\pi)(\mathcal{H}_\tau) \subset L^2_\tau(\mathbb{R}^3, \mathcal{D})$. Note that this is nontrivial since

$$L^2(\mathbb{R}^3, \mathcal{D}) \subsetneqq \mathcal{S}'(\mathbb{R}^3, \mathcal{D}) \cap L^2(\mathbb{R}^3, \mathcal{H}_f).$$

Since $H\sharp\pi \in S^{\mathbf{1}}_\tau(\varepsilon, \mathcal{L}(\mathcal{H}_f))$ we know that $\mathcal{W}(H\sharp\pi) = \mathcal{W}H\mathcal{W}\pi$ restricts to a bounded operator $\widehat{H\sharp\pi}$ in $\mathcal{L}(\mathcal{H}_\tau)$. Now suppose there is a $\psi_0 \in \mathcal{H}_\tau$ with $\varphi_0 = \mathcal{W}\pi(\psi_0) \in \mathcal{H}_\tau \setminus L^2_\tau(\mathbb{R}^3, \mathcal{D})$. Then clearly we have $\mathcal{W}H\varphi_0 \in \mathcal{H}_\tau$ and H^ε_Z would have a nontrivial symmetric extension (with domain spanned by $L^2_\tau(\mathbb{R}^3, \mathcal{D})$ and φ_0) which is a contradiction to the self-adjointness of H^ε_Z. Furthermore we now know that

$$(H^\varepsilon_Z - i)^{-1}\left(\mathcal{W}(H-i)\mathcal{W}\pi\right)\varphi = \mathcal{W}\pi\varphi, \quad \varphi \in \mathcal{H}_\tau.$$

therefore $\mathcal{W}\pi$ restricts to a bounded operator $\widehat{\pi} \in \mathcal{L}(\mathcal{H}_\tau, L^2_\tau(\mathbb{R}^3, \mathcal{D}))$. Clearly we have $\widehat{J\pi} = J\widehat{\pi}$ since $\mathcal{W}(J\pi) = \mathcal{W}J\mathcal{W}\pi$ and therefore we can drop the distinction between π and $J\pi$ resp. $\widehat{\pi}$ and $\widehat{J\pi}$ from now on.

We turn to determine the "commutator" (see remark 2.11) of $\widehat{H}$ and $\widehat{\pi}$. As we know that $H\sharp\pi \in S^{w^2}_{\tau}(\varepsilon, \mathcal{L}(\mathcal{H}_f)) \subset S^{\mathbf{1}}_{\tau}(\varepsilon, \mathcal{L}(\mathcal{H}_f))$ and also $(H\sharp\pi)^* \in S^{\mathbf{1}}_{\tau}(\varepsilon, \mathcal{L}(\mathcal{H}_f))$ it follows that

$$\left\| \widehat{H}\widehat{\pi} - \left(\widehat{H}\widehat{\pi}\right)^* \right\|_{\mathcal{L}(\mathcal{H}_f)} = \mathcal{O}(\varepsilon^\infty).$$

Next we construct a true projector which is $\mathcal{O}(\varepsilon^\infty)$-close to $\widehat{\pi}$. We know from (2.22) that $\widehat{\pi}$ is self-adjoint and its spectrum is concentrated around 0 and 1 for ε small enough, let's say in intervals I_0 and I_1 whose length is $\mathcal{O}(\varepsilon^\infty)$ and in particular smaller than $\frac{1}{2}$ for ε small enough. Therefore

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

is a true projector with

$$\begin{aligned} \|\widehat{\pi} - \Pi^\varepsilon_Z\| &= \int_{I_0} \lambda E(\mathrm{d}\lambda) + \int_{I_1} (\lambda - 1) E(\mathrm{d}\lambda) \\ &= \mathcal{O}(\varepsilon^\infty) \end{aligned}$$

where $E(\cdot)$ denotes the projection valued measure of $J\widehat{\pi}$. Finally we have

$$\begin{aligned} &\exp(-iH^\varepsilon_Z t)\Pi^\varepsilon_Z \exp(iH^\varepsilon_Z t) - \Pi^\varepsilon_Z \\ &\quad= \exp(-i\widehat{H}t)\widehat{\pi}\exp(i\widehat{H}t) - \widehat{\pi} + \mathcal{O}(\varepsilon^\infty) \\ &\quad= \int_0^t \mathrm{d}s \left(\frac{\mathrm{d}}{\mathrm{d}s} \left(\exp(-i\widehat{H}s) \right) \widehat{\pi} \exp(i\widehat{H}s) \right) \\ &\qquad + \int_0^t \mathrm{d}s \left(\exp(-i\widehat{H}s) \frac{\mathrm{d}}{\mathrm{d}s} \left(\exp(-i\widehat{H}s)\widehat{\pi} \right)^* \right) + \mathcal{O}(\varepsilon^\infty) \\ &\quad= -i \int_0^t \mathrm{d}s \left(\exp(-i\widehat{H}s) \right) \widehat{H}\widehat{\pi} \exp(i\widehat{H}s) \\ &\qquad + i \int_0^t \mathrm{d}s \left(\exp(-i\widehat{H}s) \left(\exp(-i\widehat{H}s)\widehat{H}\widehat{\pi} \right)^* \right) + \mathcal{O}(\varepsilon^\infty) \\ &\quad= -i \int_0^t \mathrm{d}s \exp(-i\widehat{H}s) \left(\widehat{H}\widehat{\pi} - \left(\widehat{H}\widehat{\pi} \right)^* \right) \exp(i\widehat{H}s) + \mathcal{O}(\varepsilon^\infty) \\ &\quad= \mathcal{O}(\varepsilon^\infty(1 + |t|)) \end{aligned}$$

where we used that $(J\widehat{\pi})^* = J\widehat{\pi}$ and the fact that taking adjoints commutes with the derivative. ■

2.2.2 Mapping to the reference space

After determining the almost invariant subspace, we want to describe the dynamics inside the subspace in a simple way. As shown in [Pa] there is a smooth isometry-valued map $U_{\mathrm{per}} : \mathbb{R}^3 \to \mathcal{U}(\mathcal{H}_f)$ such that

$$U_{\mathrm{per}}(k)^* P_{\mathrm{per}}(k) U_{\mathrm{per}}(k) = P_{\mathrm{per}}(0) =: \pi_r$$

such that U_{per} is right-τ-equivariant, i.e.

$$U_{\mathrm{per}}(k+\gamma^*) = U_{\mathrm{per}}(k)\tau(\gamma^*).$$

Clearly the dynamics of the unperturbed problem inside $P_{\mathrm{per}}\mathcal{H}_\tau$ can be described in $\mathcal{K}$ by the Hamiltonian

$$\int_{\mathbb{R}^3}^{\oplus} \mathrm{d}k \mathbf{h}_{\mathrm{per}}(k) \oplus \mathbf{0}_{\mathcal{K}_f^\perp} := \int_{\mathbb{R}^3}^{\oplus} \mathrm{d}k U_{\mathrm{per}}(k)^* H_{\mathrm{per}}(k) P_{\mathrm{per}}(k) U_{\mathrm{per}}(k)$$

where $\mathbf{h}_{\mathrm{per}}(k) \in \mathcal{L}(\mathcal{K}_f)$, i.e. $\mathbf{h}_{\mathrm{per}}(k)$ is for fixed k a $N \times N$-matrix. In the perturbed case, we have an analogous result up to errors of order $\mathcal{O}(\varepsilon^\infty)$. One starts with the observation that $u_0 : \mathbb{R}^6 \to \mathcal{U}(\mathcal{H}_f)$ given by

$$u_0(q,p) = U_{\mathrm{per}}(q - A(p)) \tag{2.23}$$

is in $S^{\mathbf{1}}_{\tau,\mathbf{1}}(\mathcal{L}(\mathcal{H}_f))$ and intertwines π and π_r (in the Moyal sense) up to order ε.

Proposition 2.12 *Let $\{E_n\}_{n\in\mathcal{I}}$ be an isolated family of bands and let Assumption (A1) be satisfied. Then there exists a unitary operator $U^\varepsilon : \mathcal{H}_\tau \to \mathcal{H}_r$ such that*

$$U^\varepsilon \Pi^\varepsilon_Z U^{\varepsilon *} = \widehat{\pi}_r =: \Pi_r$$

and $U^\varepsilon - \widehat{u} = \mathcal{O}(\varepsilon^\infty)$, where

$$u \asymp \sum_{j\geq 0} \varepsilon^j u_j \quad \text{in } S^{\mathbf{1}}(\varepsilon, \mathcal{L}(\mathcal{H}_f)).$$

Furthermore u is right τ-covariant and its principal symbol is given in (2.23).

As before we split the proof in two pieces and first construct the symbol u.

Lemma 2.13 *There is a formal symbol $u = \sum_{j\geq 0} \varepsilon^j u_j \in M^{\mathbf{1}}(\varepsilon, \mathcal{L}(\mathcal{H}_f))$ which is right τ-covariant and whose principal symbol u_0 is given in (2.23) such that* *(i)* $u^*\sharp u = \mathbf{1}$ *and* $u\sharp u^* = \mathbf{1}$,

(ii) $u\sharp\pi\sharp u^* = \pi_r$.

Proof. We construct u by induction. Clearly u_0 satisfies the conditions (i) and (ii) up to order ε and is right τ-covariant. Now suppose we have found u_j, $0 \le j \le n$ such that each $u_j \in S^{\mathbf{1}}(\mathcal{L}(\mathcal{H}_f))$ is right τ-covariant and satisfies (i) and (ii) up to order ε^{n+1}. To determine u_{n+1} we make the ansatz

$$u_{n+1} =: (a_{n+1} + b_{n+1})u_{0,} \tag{2.24}$$

with a_{n+1} hermitian and b_{n+1} anti-hermitian. For (i), we have by induction assumption

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

This gives the conditions

$$\begin{aligned} u_0 u_{n+1}^* + u_{n+1}u_0^* &= -A_{n+1}, \\ u_{n+1}^* u_0 + u_0^* u_{n+1} &= -\tilde{A}_{n+1}. \end{aligned} \tag{2.25}$$

By multiplying the first equation from left with u_0^* and the second equation with u_0^* from the right we see that they are equivalent, because

$$\varepsilon^{-(n+1)}u^{(n)*}\sharp\left(u^{(n)}\sharp u^{(n)*} - \mathbf{1}\right) = \varepsilon^{-(n+1)}(u^{(n)*}\sharp u^{(n)} - \mathbf{1})\sharp u^{(n)*}$$

and the principal symbol of the l.h.s. is $u_0^*A_{n+1}$ whereas the principal symbol of the r.h.s. is $A_{n+1}u_0^*$. If we insert (2.24) into (2.25) we find that $a_{n+1} = -\frac{1}{2}A_{n+1}$ since A_{n+1} is hermitian (because $u^{(n)}\sharp u^{(n)*} - \mathbf{1}$ is hermitian) whereas no constraint is put on b_{n+1}, which is now determined in order to satisfy (ii). If we define $\omega^{(n)} := u^{(n)} + \varepsilon^{n+1}a_{n+1}u_0$ then we have

$$\omega^{(n)}\sharp\pi\sharp\omega^{(n)*} - \pi_r = \varepsilon^{n+1}B_{n+1} + \mathcal{O}(\varepsilon^{n+2})$$

and therefore

$$b_{n+1}u_0\pi_0u_0^* + u_0\pi u_0^* b_{n+1}^* = -B_{n+1}. \tag{2.26}$$

The left hand side is just $[b_{n+1}, \pi_r]$ and a solution to (2.26) is given by

$$b_{n+1} = [\pi_r, B_{n+1}],$$

provided that the so-defined b_{n+1} is indeed anti-hermitian. This is the case if B_{n+1} is hermitian and off-diagonal with respect to π_r. The Hermiticity of B_{n+1} is clear from its definition. Furthermore we have

$$\begin{aligned}&(1-\pi_r)B_{n+1}(1-\pi_r)\\ &= \varepsilon^{-(n+1)}(1-\pi_r)\sharp\left(\omega^{(n)}\sharp\pi\sharp\omega^{(n)*}-\pi_r\right)\sharp(1-\pi_r)+\mathcal{O}(\varepsilon)\\ &= \varepsilon^{-(n+1)}(1-\pi_r)\sharp\omega^{(n)}\sharp\pi\sharp\omega^{(n)*}\sharp(1-\pi_r)+\mathcal{O}(\varepsilon).\end{aligned}$$

Since we know that

$$(1-\pi_r)=\omega^{(n)}\sharp(1-\pi)\sharp\omega^{(n)*}+\varepsilon^{n+1}B_{n+1}+\mathcal{O}(\varepsilon^{n+2})$$

and $\omega^{(n)}\sharp\omega^{(n)*}=1+\mathcal{O}(\varepsilon^{n+2})$ this leads to

$$\begin{aligned}&(1-\pi_r)B_{n+1}(1-\pi_r)\\ &= \varepsilon^{-(n+1)}\varepsilon^{2(n+1)}B_{n+1}(\omega^{(n)}\sharp\pi\sharp\omega^{(n)*})B_{n+1}+\mathcal{O}(\varepsilon)\\ &= 0+\mathcal{O}(\varepsilon).\end{aligned}$$

Finally we have

$$B_{n+1}=\varepsilon^{-(n+1)}\left(\omega^{(n)}\sharp(1-\pi)\sharp\omega^{(n)*}-(1-\pi_r)\right)+\mathcal{O}(\varepsilon)$$

because $\omega^{(n)}\sharp\omega^{(n)*}=1+\mathcal{O}(\varepsilon^{n+2})$ and therefore an analogous argument shows

$$\pi_r B_{n+1}\pi_r=0+\mathcal{O}(\varepsilon).$$

Finally $u\in M^{\mathbf{1}}(\varepsilon,\mathcal{L}(\mathcal{H}_f))$ is clear from construction and the fact that it is right covariant follows from the fact that A_{n+1}, B_{n+1} are periodic and u_0 is right covariant. ■

Now we give the proof .

Proof. (of proposition 2.12) By resummation we get a (right τ-covariant) symbol $u\in S^{\mathbf{1}}(\varepsilon,\mathcal{L}(\mathcal{H}_f))$. Its quantization yields a bounded operator $\widehat{u}\in\mathcal{L}(\mathcal{H}_\tau,\mathcal{H}_r)$ that satisfies

(*i*) $\widehat{u}\widehat{u}^*=\mathbf{1}_{\mathcal{H}_r}+\mathcal{O}(\varepsilon^\infty)$ and $\widehat{u}^*\widehat{u}=\mathbf{1}_{\mathcal{H}_\tau}+\mathcal{O}(\varepsilon^\infty)$

(*ii*) $\widehat{u}\Pi^\varepsilon_Z\widehat{u}^*=\Pi_r+\mathcal{O}(\varepsilon^\infty)$.

Now one can first modify $\widehat{u}$ to get a unitary operator. One observes that $\widehat{u}^*\widehat{u}\in\mathcal{L}(\mathcal{H}_\tau)$ is a positive, self-adjoint operator that is $\mathcal{O}(\varepsilon^\infty)$-close to the identity. Therefore

$$\widetilde{U}^\varepsilon:=\widehat{u}(\widehat{u}^*\widehat{u})^{-\frac{1}{2}}$$

defines a unitary operator which is $\mathcal{O}(\varepsilon^\infty)$-close to $\widehat{u}$. Finally one defines $W^\varepsilon \in \mathcal{L}(\mathcal{H}_r)$ by the so-called Nagy formula as

$$W^\varepsilon = (\mathbf{1}_{\mathcal{H}_r} - (\widetilde{U}^\varepsilon \Pi_Z^\varepsilon \widetilde{U}^{\varepsilon *} - \Pi_r)^2)^{-\frac{1}{2}} (\Pi_r \widetilde{U}^\varepsilon \Pi_Z^\varepsilon \widetilde{U}^{\varepsilon *} + (\mathbf{1}_{\mathcal{H}_r} - \Pi_r)(\mathbf{1}_{\mathcal{H}_r} - \widetilde{U}^\varepsilon \Pi_Z^\varepsilon \widetilde{U}^{\varepsilon *})).$$

W^ε is a unitary operator which is $\mathcal{O}(\varepsilon^\infty)$-close to the identity and

$$W^\varepsilon \widetilde{U}^\varepsilon \Pi_Z^\varepsilon \widetilde{U}^{\varepsilon *} W^{\varepsilon *} = \Pi_r,$$

i.e. $U^\varepsilon := W^\varepsilon \widetilde{U}^\varepsilon$ is a unitary operator with the desired properties of proposition 2.12. ■

2.2.3 The effective Hamiltonian

Now we proceed with the final step in space-adiabatic perturbation theory, namely to unitarily transform the Hamiltonian onto the reference space. While formally the definition $h = u \sharp H \sharp u^*$ seems straightforward, we project H on the relevant subspace before rotating it to the reference space since $H \in S^w(\varepsilon, \mathcal{L}(\mathcal{D}, \mathcal{H}_f))$ and $u^* \in S^{\mathbf{1}}(\varepsilon, \mathcal{L}(\mathcal{H}_f))$ are formally not compatible. For the computation it will turn out useful to introduce the kinetic momentum $\widetilde{q} : \mathbb{R}^6 \to \mathbb{R}^3$ by

$$\widetilde{q}(q, p) = q - A(p).$$

Note that with this notation we have $u_0 = U_{\text{per}} \circ \widetilde{q}$, $\pi_0 = P_{\text{per}} \circ \widetilde{q}$ etc. It is also useful to define ∇f for any function $f : \mathbb{R}^n \to \mathbb{R}^m$ as the Jacobian matrix, i.e.

$$(\nabla f)_{i,j} = \partial_j f_i.$$

Note that with that convention, the chain rule becomes $\nabla(f \circ g) = ((\nabla f) \circ g) \nabla g$ and the gradient of a scalar-valued function is seen as a row vector. We also emphasize, that for vector operations as the scalar or the cross products we always write operations, i.e. $\cdot$ and $\times$, explicitly, whereas for matrix multiplication we just put matrices behind each other.
Proof. (of theorem 2.6) We define $\mathbf{h} \in M^{\mathbf{1}}_{\tau \equiv \mathbf{1}}(\varepsilon, \mathcal{L}(\mathcal{K}_f))$ by

$$\mathbf{h} \oplus \mathbf{0}_{\mathcal{K}_f^\perp} := u \sharp H \sharp \pi \sharp u^* \in M^{\mathbf{1}}_{\tau \equiv \mathbf{1}}(\varepsilon, \mathcal{L}(\mathcal{H}_f)).$$

First note that $\mathbf{h}$ is well-defined by construction because

$$u \sharp H \sharp \pi \sharp u^* = \pi_r \left(u \sharp H \sharp \pi \sharp u^* \right) \pi_r.$$

Since $H\sharp\pi$ and u are in $M^{\mathbf{1}}(\varepsilon,\mathcal{L}(\mathcal{H}_f))$ and τ-covariant resp. right covariant it follows that $\mathbf{h}\in M^{\mathbf{1}}_{\tau\equiv\mathbf{1}}(\varepsilon,\mathcal{L}(\mathcal{K}_f))$. In particular its quantization $\widehat{\mathbf{h}}$ is in $\mathcal{L}(\mathcal{K})$. Clearly $[\widehat{\mathbf{h}}\oplus\mathbf{0}_{\mathcal{K}^\perp},\Pi_r]=0$ because $\Pi_r=\mathbf{1}_{\mathcal{K}}\oplus\mathbf{0}_{\mathcal{K}^\perp}$. Furthermore we have

$$\begin{aligned}
&\exp(-i\widehat{H}t)\Pi^\varepsilon_Z-U^\varepsilon\left(\exp(-i\widehat{\mathbf{h}}t)\oplus\mathbf{0}_{\mathcal{K}^\perp}\right)U^{\varepsilon*}\\
&=\int_0^t\mathrm{d}s\frac{\mathrm{d}}{\mathrm{d}s}\left(\exp(-i\widehat{H}s)\widehat{\pi}U^\varepsilon\left(\exp(-i\widehat{\mathbf{h}}(t-s))\oplus\mathbf{0}_{\mathcal{K}^\perp}\right)\right)U^{\varepsilon*}+\mathcal{O}(\varepsilon^\infty)\\
&=-i\int_0^t\mathrm{d}s\exp(-i\widehat{H}s)\left(\widehat{H}\widehat{\pi}U^\varepsilon-U^\varepsilon\left(\widehat{\mathbf{h}}\oplus\mathbf{0}_{\mathcal{K}^\perp}\right)\right)\left(\exp(-i\widehat{\mathbf{h}}s)\oplus\mathbf{0}_{\mathcal{K}^\perp}\right)U^{\varepsilon*}\\
&\quad+\mathcal{O}(\varepsilon^\infty).
\end{aligned}$$

On the other hand $H\sharp\pi\sharp u=u\sharp\left(\mathbf{h}\oplus\mathbf{0}_{\mathcal{K}_f^\perp}\right)$ by construction and $\widehat{H}\widehat{\pi}=\widehat{H\sharp\pi}$ therefore

$$\left(\widehat{H}\widehat{\pi}U^\varepsilon-U^\varepsilon\left(\widehat{\mathbf{h}}\oplus\mathbf{0}_{\mathcal{K}^\perp}\right)\right)=\mathcal{O}(\varepsilon^\infty)$$

and (2.14) holds. Theorem 2.6 now follows by observing that

$$\mathbf{h}_0\oplus\mathbf{0}_{\mathcal{K}_f^\perp}:=u_0H_0\pi_0u_0^*.$$

■

In the case of a single eigenvalue, i.e. $E_n(k)=E_*(k)$, $k\in M^*, n=1,\dots,N$, we also compute the subprincipal symbol $\mathbf{h}_1$. Note that this case typically occurs if V_Γ is inversion-symmetric and the family $\{E_n\}_{n\in\mathcal{I}}$ is two-fold degenerate, i.e. $N=2$.

Proof. (of corollary 2.8) By Moyal-multiplying the defining equation of $\mathbf{h}$ from left with u^* we have

$$u^*\sharp\left(\mathbf{h}\oplus\mathbf{0}_{\mathcal{K}_f^\perp}\right)=H\sharp\pi\sharp u^*.$$

Furthermore, we know that $\pi\sharp u^*=u^*\pi_r$. Note that the distinction between symbols with values in $\mathcal{L}(\mathcal{H}_f,\mathcal{D})$ and their extensions to $\mathcal{L}(\mathcal{H}_f)$ may be neglected because the derivatives in $\mathcal{L}(\mathcal{H}_f)$ are just the extensions of the corresponding derivatives in $\mathcal{L}(\mathcal{H}_f,\mathcal{D})$. Therefore $\mathbf{h}_1$ satisfies (with $H_1=0$)

$$\begin{aligned}
&\mathbf{h}_1\oplus\mathbf{0}_{\mathcal{K}_f^\perp} &(2.27)\\
&=u_0\left(-u_1^*\left(\mathbf{h}_0\oplus\mathbf{0}_{\mathcal{K}_f^\perp}\right)+\frac{i}{2}\{u_0,\mathbf{h}_0\oplus\mathbf{0}_{\mathcal{K}_f^\perp}\}+H_0u_1^*\pi_r-\frac{i}{2}\{H_0,u_0^*\pi_r\}\right)\\
&=-u_0u_1^*\widetilde{E}_*\pi_r+\frac{i}{2}u_0\{u_0^*,\widetilde{E}_*\}\pi_r+u_0H_0u_1^*\pi_r-\frac{i}{2}\{H_0,u_0^*\pi_r\}
\end{aligned}$$

with $\widetilde{E}_*(q,p) = E_* \circ \widetilde{q}(q,p) + \phi(p)$. Obviously we can multiply the equation from right and left with π_r without changing the left hand side, therefore

$$\begin{aligned}
\mathbf{h}_1 \oplus \mathbf{0}_{\mathcal{K}_f^\perp} &= \frac{i}{2}\pi_r u_0 \left(\{u_0^*, \widetilde{E}_*\pi_r\} - \{H_0, u_0^*\pi_r\}\right) \\
&= -\frac{i}{2}\pi_r u_0\{H_0 - \widetilde{E}_*\mathbf{1}_{\mathcal{H}_f}, u_0^*\}\pi_r - i\pi_r u_0\{\widetilde{E}_*\mathbf{1}_{\mathcal{H}_f}, u_0^*\}\pi_r
\end{aligned}$$

because the two other terms cancel each other due to $\pi_r u_0 H_0 = \widetilde{E}_*\pi_r u_0$.

Now we turn to compute $\mathbf{h}_1$ in terms of eigenfunctions of the unperturbed Hamiltonian. We have

$$\begin{aligned}
&\{H_0 - \widetilde{E}_*\mathbf{1}_{\mathcal{H}_f}, u_0^*\} \\
&\quad= \nabla_q\left((H_{\mathrm{per}} - E_*)\circ\widetilde{q}\right)\cdot\nabla_p\left(U_{\mathrm{per}}^*\circ\widetilde{q}\right) - \nabla_p\left((H_{\mathrm{per}} - E_*)\circ\widetilde{q}\right)\cdot\nabla_q\left(U_{\mathrm{per}}^*\circ\widetilde{q}\right) \\
&\quad= \left(\nabla\left(H_{\mathrm{per}} - E_*\right)\circ\widetilde{q}\right)\left(\nabla A - (\nabla A)^\top\right)\left(\nabla^\top U_{\mathrm{per}}^*\circ\widetilde{q}\right)
\end{aligned}$$

where ∇A is the Jacobian of A. One has furthermore $\left(\nabla A - (\nabla A)^\top\right)x = B\times x$ for any $x\in\mathbb{R}^3$ where $B := \nabla\times A$ is the magnetic field and $\nabla U_{\mathrm{per}}^* = \sum_{j\le N}\left\langle\chi_j,\cdot\right\rangle\nabla\psi_j$, therefore the ν,μ element of the first term in (2.27) contributes to (2.15) with

$$\begin{aligned}
&-\frac{i}{2}\left\langle\psi_n\circ\widetilde{k}, \left(\nabla(H_{\mathrm{per}} - E_*)\circ\widetilde{q}\right)\cdot B\times\left(\nabla_k\psi_m\circ\widetilde{q}\right)\right\rangle \\
&\quad= -\frac{i}{2}B\cdot\langle\nabla_k\psi_n, \times(H_{\mathrm{per}} - E_*)\nabla_k\psi_m\rangle\circ\widetilde{q}
\end{aligned}$$

where we used the vector equality $a\cdot(b\times c) = -b\cdot(a\times c)$ (note that B is scalar-valued) and shifted the gradient on $H_{\mathrm{per}} - E_*$ to ψ_n by observing that

$$\begin{aligned}
0 &= \nabla\left\langle\psi_n, \left(H_{\mathrm{per}} - E_*\right)\varphi\right\rangle \\
&= \langle\nabla\psi_n, (H_{\mathrm{per}} - E_*)\varphi\rangle + \langle\psi_n, \nabla(H_{\mathrm{per}} - E_*)\varphi\rangle
\end{aligned}$$

for all $\varphi\in\mathcal{D}$. The second term in (2.27) can be manipulated analogously and contributes to (2.15) with

$$i\left(\nabla\phi - (\nabla E_*\circ\widetilde{q})\times B\right)\cdot\langle\psi_n, \nabla_k\psi_m\rangle\circ\widetilde{q}.$$

■

2.3 Semiclassical limit

All the results of the last sections are purely quantum mechanical, symbols were used only as a tool. In this section, we show how to approximate the quantum mechanical time evolution of observables which are quantizations of symbols by a classical Hamiltonian system on an appropriate phase space. As a start, we sketch the idea. The time evolution under the Hamiltonian $\widehat{\mathbf{h}}$ of an observable $\widehat{\mathbf{a}}$ with $\mathbf{a} \in S(\mathcal{L}(\mathcal{K}_f))$ in the reference space, i.e. the quantity

$$\widehat{\mathbf{a}}(t) = \exp(i\widehat{\mathbf{h}}t/\varepsilon)\widehat{\mathbf{a}}\exp(-i\widehat{\mathbf{h}}t/\varepsilon)$$

satisfies the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\widehat{\mathbf{a}}(t) = \frac{i}{\varepsilon}(\widehat{\mathbf{h}}\widehat{\mathbf{a}}(t) - \widehat{\mathbf{a}}(t)\widehat{\mathbf{h}}). \tag{2.28}$$

Note that since we want to consider time periods of order $\mathcal{O}(\varepsilon^{-1})$, we have chosen $\exp(i\widehat{\mathbf{h}}t/\varepsilon)$ instead of $\exp(i\widehat{\mathbf{h}}t)$ as explained in the introduction of this chapter. Formally the time derivative in (2.28) is expected to commute with quantization, therefore we can translate (2.28) on the level of symbols and obtain the differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{a}(t) = \frac{i}{\varepsilon}(\mathbf{h}\sharp\mathbf{a}(t) - \mathbf{a}(t)\sharp\mathbf{h}). \tag{2.29}$$

If $\mathbf{a}$ and $\mathbf{h}$ are multiples of the identity, the right hand side equals $\{\mathbf{h}, \mathbf{a}\}$ up to order $\mathcal{O}(\varepsilon^2)$, therefore (2.29) is (up to order $\mathcal{O}(\varepsilon^2)$) solved by $\mathbf{a}(t) = \mathbf{a} \circ \Phi^t$, where Φ^t is the flow generated by the scalar Hamiltonian $\mathbf{h}$.

Dealing with matrix-valued symbols changes the picture slightly. Most important, due to the prefactor $\frac{i}{\varepsilon}$ on the right hand side of (2.29), we must have $[\mathbf{h}_0, \mathbf{a}(t)] = 0 \quad \forall t \in \mathbb{R}$ which is in general only satisfied if $\mathbf{h}_0$ is a scalar multiple of the identity, i.e. in the case of a single (maybe degenerate) eigenvalue band. Since lemma 2.2 tells us that an isolated family cannot consist of a single non-degenerate band, we restrict ourselves to the case of a space-inversion-symmetric potential V_Γ and $N = 2$. Then corollary 2.3 ensures us that each eigenvalue is indeed globally two-fold degenerate and gives also explicit information about the corresponding pair of eigenfunctions. Second, the right hand side of (2.29) contains an additional term $[\mathbf{h}_1, \mathbf{a}(t)]$. Since symbols $\mathbf{a}$ and $\mathbf{b}$ with self-adjoint values in $\mathcal{L}(\mathcal{K}_f)$ with $\mathcal{K}_f \cong \mathbb{C}^2$ can always be written in the form $\mathbf{a} = a_0\mathbf{1}_{\mathcal{K}_f} + a \cdot \boldsymbol{\sigma}_{\mathcal{K}_f}$ with $a_0 \in \mathbb{R}$, $a \in \mathbb{R}^3$, $\boldsymbol{\sigma}_{\mathcal{K}_f}$ defined via the isomorphy $\mathcal{L}(\mathcal{K}_f) \cong \mathcal{L}(\mathbb{C}^2)$, one obtains

$$[\mathbf{a}, \mathbf{b}] = i(a \times b) \cdot \boldsymbol{\sigma}_{\mathcal{K}_f}$$

and uses this relation to go to scalar equations.

The strategy in this section is the following: In subsection 2.3.1 we perform the semiclassical limit in the reference space. To this end, we introduce, following [Teu], a correspondence between $\mathcal{L}(\mathbb{C}^2)$-valued symbols on the phase space $\mathbb{R}^6$ and scalar-valued symbols on the extended phase space $\mathbb{R}^6 \times S^2$ where S^2 is the unit sphere in $\mathbb{R}^3$. The points on S^2 can be interpreted as the spin of the particle. We show that an appropriate ε-dependent flow Φ^t_ε on $\mathbb{R}^6 \times S^2$ generates a time evolution of symbols that satisfies (2.29) and (after quantization) (2.28) up to order $\mathcal{O}(\varepsilon)$. If $\mathbf{a}$ is a multiple of the identity, we can improve the error to order $\mathcal{O}(\varepsilon^2)$. In subsection 2.3.2 we show how to translate the results in the reference space back to the Zak representation. The effective equations of motion in Zak representation that approximate the quantum mechanical time evolution up to order $\mathcal{O}(\varepsilon^2)$ are

$$\begin{aligned} \dot{\tilde{q}} &= -\nabla_p(\phi(p) - \varepsilon B(p)\cdot\mathcal{M}(\tilde{q},n)) + \varepsilon\dot{p}\times B(p) \\ \dot{p} &= \nabla_{\tilde{q}}(E_*(\tilde{q}) - \varepsilon B(\Pi)\cdot\mathcal{M}(\tilde{q},n)) + \varepsilon\Omega_{\mathcal{A}}(\tilde{q},n)\times\dot{\tilde{q}} + \varepsilon\left(\nabla_n\mathcal{A}(\tilde{q},n)\right)\cdot\dot{n} \\ \dot{n} &= n\times\widetilde{\Omega}(\tilde{q},p) \end{aligned} \tag{2.30}$$

on the phase space $\mathbb{R}^6 \times S^2$ where S^2 is the unit sphere in $\mathbb{R}^3$. The terms $\mathcal{M}$ and $\mathcal{A}$ are given in corollary 2.8 and definition 2.16 whereas $\Omega_{\mathcal{A}}(k,n) := \nabla_k \times \mathcal{A}(k,n)$ and $\widetilde{\Omega}$ is given in (2.36). If we define $\tilde{\Phi}^{t,\varepsilon}_Z$ to be the flow of (2.30) and

$$\Phi^{t,\varepsilon}_Z(q,p,n) = \tilde{\Phi}^{t,\varepsilon}_Z(q - A(p),p,n) + (A\circ\tilde{\Phi}^{t,\varepsilon}_{Z,p}(q - A(p)),0,0), \tag{2.31}$$

we have the following theorem.

Theorem 2.14 *Let V_Γ be inversion-symmetric and $|\mathcal{I}| = 2$, i.e. E is an isolated two-fold degenerate Bloch band, and $\Phi^{t,\varepsilon}_Z$ be defined as in (2.31). Let furthermore $b \in C^\infty_b(\mathbb{R}^6 \times S^2, \mathbb{C})$ and*

$$\mathbf{b}_\varepsilon(t) := \mathcal{W}(2\int_{S^2} d\lambda(n) b\circ\Phi^{t,\varepsilon}_Z(\cdot,\cdot,n)\tilde{\mathbf{\Delta}}(\cdot,\cdot,n))$$

with $\tilde{\mathbf{\Delta}} : \mathbb{R}^6 \times S^2 \to \mathcal{L}(\mathcal{H}_f)$ defined in (2.47) and $\mathbf{b}_\varepsilon := \mathbf{b}_\varepsilon(0)$. Then we have

$$\exp(iH^\varepsilon_Z t/\varepsilon)\widehat{\mathbf{b}}\exp(-iH^\varepsilon_Z t/\varepsilon) - \widehat{\mathbf{b}_0(t)} = \mathcal{O}(\varepsilon)$$

uniformly for any finite time interval, and, if b is independent of n,

$$\exp(iH^\varepsilon_Z t/\varepsilon)\widehat{\mathbf{b}}\exp(-iH^\varepsilon_Z t/\varepsilon) - \widehat{\mathbf{b}_\varepsilon(t)} = \mathcal{O}(\varepsilon^2).$$

If we restrict our considerations to $\mathcal{O}(\varepsilon)$ and scalar-valued $\mathbf{b}$ (i.e. b independent of n), then we can even translate the result of theorem 2.14 back to the physical space. In [Teu] it is shown that the Zak transform is for a certain class of symbols equivalent to exchange the arguments q and p. If $\tilde{\Phi}^t$ is the flow of the equations

$$\begin{aligned} \dot{q} &= \nabla E_*(\pi) \\ \dot{\pi} &= -\nabla\phi(q) \end{aligned} \tag{2.32}$$

and

$$\Phi^t(q,p) = \tilde{\Phi}^t(q, p - A(q)) + (0, A \circ \tilde{\Phi}^t_q(q, q - A(p)), 0), \tag{2.33}$$

we have the following corollary.

Corollary 2.15 *Let V_Γ be inversion-symmetric and $|\mathcal{I}| = 2$, i.e. E_* is an isolated two-fold degenerate energy band and Φ^t be defined as in (2.33). Let furthermore $b \in C_b^\infty(\mathbb{R}^6, \mathbb{C})$ be Γ^*-periodic in the second argument, i.e. $b(q, p + \gamma^*) = b(q,p)$. Then we have*

$$\Pi^\varepsilon \left(\exp(iH^\varepsilon t/\varepsilon)\widehat{b}\exp(-iH^\varepsilon t/\varepsilon) - \mathcal{W}(b \circ \Phi^t) \right) \Pi^\varepsilon = \mathcal{O}(\varepsilon)$$

uniformly for any finite time interval, where the Weyl quantization is in the sense of

$$\widehat{b} = b(-i\nabla_x, \varepsilon x)$$

and

$$\Pi_\varepsilon := \left(\mathcal{U}^{-1} \otimes \mathbf{1}_{\mathbb{C}^4}\right) \Pi^\varepsilon_Z \left(\mathcal{U} \otimes \mathbf{1}_{\mathbb{C}^4}\right).$$

Proof. We identify b with $b : \mathbb{R}^6 \times S^2 \to \mathbb{C}$, $(q,p,n) \mapsto b(q,p)$. Then theorem 2.14 tells us that

$$\exp(iH^\varepsilon_Z t/\varepsilon)\widehat{\mathbf{b}}\exp(-iH^\varepsilon_Z t/\varepsilon) - \mathcal{W}(2\int_{S^2} \mathrm{d}\lambda(n) b \circ \Phi^{t,0}_Z(\cdot,\cdot,n)\tilde{\mathbf{\Delta}}(q,p,n)) = \mathcal{O}(\varepsilon)$$

in Zak representation. Since b is scalar-valued and Φ^t doesn't depend on n either, b and $b \circ \Phi^t$ are independent of n and can be taken outside the integral, i.e.

$$\begin{aligned} \widehat{\mathbf{b}} &= \mathcal{W}(b2\int_{S^2} \mathrm{d}\lambda(n)\tilde{\mathbf{\Delta}}(q,p,n)) \\ &= \mathcal{W}(b\pi) \\ &= \widehat{b\mathbf{1}_{\mathcal{H}_f}}\Pi^\varepsilon_Z + \mathcal{O}(\varepsilon) \end{aligned}$$

and

$$\begin{aligned}
&\mathcal{W}(2\int_{S^2} \mathrm{d}\lambda(n) b\circ\Phi_Z^{t,0}(\cdot,\cdot,n)\tilde{\mathbf{\Delta}}(q,p,n)) \\
&= \mathcal{W}(b\circ\Phi_Z^{t,0} 2\int_{S^2} \mathrm{d}\lambda(n)\tilde{\mathbf{\Delta}}(q,p,n)) \\
&= \widehat{b\circ\Phi_Z^{t,0}\mathbf{1}}_{\mathcal{H}_f}\Pi_Z^\varepsilon + \mathcal{O}(\varepsilon).
\end{aligned}$$

Note that we used

$$\begin{aligned}
&2\int_{S^2} \mathrm{d}\lambda(n)\tilde{\mathbf{\Delta}}(q,p,n) \\
&= u\sharp 2\int_{S^2} \mathrm{d}\lambda(n)\mathbf{\Delta}(q,p,n)\sharp u^* \\
&= u\sharp\pi_r\sharp u^* = \pi.
\end{aligned}$$

Now in [Teu] it is proved that

$$b(x,-i\varepsilon\nabla_x) = \mathcal{U}b(-i\nabla_x,\varepsilon x)\mathcal{U}^{-1}$$

for scalar-valued symbols b that are additionally Γ^*-periodic in the first argument. Then our result follows directly by inserting $\mathcal{U}^{-1}\mathcal{U}$ between all the factors in the statement of theorem 2.14. ■

2.3.1 Semiclassical limit in the reference space

First we turn to define a correspondence between scalar-valued functions on $\mathbb{R}^d\times S^2$ and $\mathcal{L}(\mathcal{K}_f)$-valued functions on $\mathbb{R}^d$. In the following, we always use boldface letters to denote the latter ones.

Definition 2.16 *We associate to each smooth function $\mathbf{a}:\mathbb{R}^d\to\mathcal{L}(\mathcal{K}_f)\cong\mathcal{L}(\mathbb{C}^2)$ the function $a:\mathbb{R}^d\times S^2\to\mathbb{C}$ given by*

$$a(q,p,n) = tr(\mathbf{a}(q,p)\mathbf{\Delta}(n)) \tag{2.34}$$

with $\mathbf{\Delta}(n)\in\mathcal{L}(\mathcal{K}_f)$ given by

$$\mathbf{\Delta}_{\nu,\mu}(n) := \frac{1}{2}\delta_{\nu,\mu} + \sqrt{\frac{3}{4}}n\cdot\boldsymbol{\sigma}_{\nu,\mu}$$

and vice versa to each smooth function $a : \mathbb{R}^d \times S^2 \to \mathbb{C}$ the function $\mathbf{a} : \mathbb{R}^d \to \mathcal{L}(\mathcal{K}_f)$ given by

$$\mathbf{a}(q,p) = 2\int_{S^2} d\lambda(n) a(q,p,n) \boldsymbol{\Delta}(n) \tag{2.35}$$

where λ denotes the normalized Lebesgue measure on S^2. Furthermore, the Weyl quantization $\widehat{a}$ of a is defined as $\widehat{\mathbf{a}}$.

We left d undetermined since we are using this correspondence for symbols (i.e. $d = 6$) as well as for quantities depending on the crystal momentum k (i.e. $d = 3$), e.g. for $\mathcal{A}$ as defined in (2.8). Note that the two operations (2.34) and (2.35) invert each other and that the symbol $\boldsymbol{\sigma}$ becomes the function $(q,p,n) \mapsto \sqrt{3}n$ (see [Teu]).

Obviously we have

$$\begin{aligned} h_0(q,p,n) &= \operatorname{tr}(\mathbf{h}_0(q,p)\boldsymbol{\Delta}(n)) \\ &= E_*(q - A(p)) \end{aligned}$$

independent of n because $\mathbf{h}_0$ is a scalar multiple of the identity and that

$$h_1(q,p,n) = -F_{\mathrm{Lor}}(\widetilde{q},p) \cdot \mathcal{A}(\widetilde{q},n) - B(p) \cdot \mathcal{M}(\widetilde{q},n).$$

Alternatively, by definition, we can write h_1 also in the form

$$\begin{aligned} h_1(q,p,n) &= \operatorname{tr}(\mathbf{h}_1(q,p)\boldsymbol{\Delta}(n)) \\ &= \frac{1}{2}\operatorname{tr}(\mathbf{h}_1(q,p)) - \frac{1}{2}\Omega(q,p) \cdot n \end{aligned} \tag{2.36}$$

with

$$\Omega(q,p) := -\sqrt{3}\operatorname{tr}\left(\mathbf{h}_1(q,p)\boldsymbol{\sigma}_{\mathcal{K}_f}\right)$$

where $\boldsymbol{\sigma}_{\mathcal{K}_f}$ is defined as

$$\left(\boldsymbol{\sigma}_{\mathcal{K}_f}\right)_{\nu,\mu} = \boldsymbol{\sigma}_{\nu,\mu}, \quad \nu,\mu = 1,2.$$

Now we turn to the derivation of the Hamiltonian equations. A natural candidate for the flow $\Phi_r^{t,\varepsilon}$ such that $\mathbf{a}(t) = 2\int_{S^2} \mathrm{d}\lambda(n) a \circ \Phi_r^{t,\varepsilon}(q,p,n)\Delta(n)$ satisfies (2.29) up to order $\mathcal{O}(\varepsilon^2)$ is the Hamiltonian flow of

$$h^\varepsilon(q,p,n) = E(q - A(p)) - \varepsilon\frac{\sqrt{3}}{2} n \cdot \Omega(q,p),$$

on $\mathbb{R}^6 \times S^2$, i.e. of $h(q,p,n)$ up to order $\mathcal{O}(\varepsilon)$. To be precise, we recall that S^2 is a symplectic manifold if one uses the area two-form to define the symplectic structure. The corresponding Poisson brackets for functions on S^2 yield in particular

$$\{a \cdot n, n\}_{S^2} = \frac{1}{\sqrt{3}} a \times n.$$

As the symplectic structure on $\mathbb{R}^6 \times S^2$ is

$$\{\cdot,\cdot\}_{\mathbb{R}^6\times S^2} := \{\cdot,\cdot\}_{\mathbb{R}^6} + \frac{1}{\varepsilon}\{\cdot,\cdot\}_{S^2}, \tag{2.37}$$

we derive the Hamiltonian equations corresponding to $h^\varepsilon(q,p,n)$ as

$$\begin{aligned} \dot{q} &= -\nabla_p h^\varepsilon(q,p,n) \\ \dot{p} &= \nabla_q h^\varepsilon(q,p,n) \\ \dot{n} &= n \times \Omega(q,p). \end{aligned} \tag{2.38}$$

To simplify the translation to the physical space in the next section, we introduce the diffeomorphism $F : \mathbb{R}^6 \times S^2$ as

$$F(q,p,n) = (q - A(p), p, n) \tag{2.39}$$

with the kinetic momentum $\widetilde{q} = q - A(p)$ and compute the vector field corresponding to the flow $\tilde{\Phi}_r^{t,\varepsilon} = F \circ \Phi_r^{t,\varepsilon} \circ F^{-1}$ which reads explicitly

$$\tilde{\Phi}_r^{t,\varepsilon}(\widetilde{q},p,n) = \Phi_r^{t,\varepsilon}(\widetilde{q} + A(p), p, n) - \left(A \circ \Phi_{r,p}^{t,\varepsilon}(\widetilde{q} + A(p), p, n), 0, 0\right).$$

We get the equations

$$\begin{aligned} \dot{\widetilde{q}} &= -\nabla\phi(p) + \dot{p} \times B(p) \\ &\quad +\varepsilon\nabla_p \left(F_{\mathrm{Lor}}(\widetilde{q},p) \cdot \mathcal{A}(\widetilde{q},n) + B(p) \cdot \mathcal{M}(\widetilde{q},n)\right) \\ \dot{p} &= \nabla E(\widetilde{q}) - \varepsilon\nabla_{\widetilde{q}} \left(F_{\mathrm{Lor}}(\widetilde{q},p) \cdot \mathcal{A}(\widetilde{q},n) + B(p) \cdot \mathcal{M}(\widetilde{q},n)\right) \\ \dot{n} &= n \times \widetilde{\Omega}(\widetilde{q},p). \end{aligned} \tag{2.40}$$

with $\widetilde{\Omega}(\widetilde{q},p) = \Omega(q - A(p), p)$. The second and the last equation in (2.40) can easily be derived from the corresponding equations in (2.38) (recall the definition of Ω), whereas the first one comes from

$$\begin{aligned} \dot{\widetilde{q}} &= \dot{q} - \dot{p}\,(\nabla A)^\top(p) \\ &= -\nabla\phi(p) + \nabla E(\widetilde{q})\nabla A(p) \\ &\quad -\varepsilon\nabla_{\widetilde{q}} \left(F_{\mathrm{Lor}}(\widetilde{q},p) \cdot \mathcal{A}(\widetilde{q},n) + B(p) \cdot \mathcal{M}(\widetilde{q},n)\right)\nabla A(p) \\ &\quad +\varepsilon\nabla_p \left(F_{\mathrm{Lor}}(\widetilde{q},p) \cdot \mathcal{A}(\widetilde{q},n) + B(p) \cdot \mathcal{M}(\widetilde{q},n)\right) - \dot{p}\,(\nabla A)^\top(p) \\ &= -\nabla\phi(p) + \dot{p}(\nabla A(p) - (\nabla A)^\top(p)) \\ &\quad +\varepsilon\nabla_p \left(F_{\mathrm{Lor}}(\widetilde{q},p) \cdot \mathcal{A}(\widetilde{q},n) + B(p) \cdot \mathcal{M}(\widetilde{q},n)\right) \end{aligned}$$

Now we turn to prove that the flow of (2.38) (or equivalently the one of (2.40)) can be used to approximate the time evolution of observables. Indeed, for observables a which are independent of n (i.e. $\mathbf{a}$ is a multiple of the identity) we have the following result:

Proposition 2.17 *Let $\Phi_r^{t,\varepsilon}$ be the solution flow of (2.38) and $a \in C_b^\infty(\mathbb{R}^6 \times S^2, \mathbb{C})$ independent of n. Then*

$$\mathbf{a}(t) := 2 \int_{S^2} d\lambda(n) a \circ \Phi_r^{t,\varepsilon}(\cdot, \cdot, n) \mathbf{\Delta}(n), \quad t \in \mathbb{R}$$

is in $S^{\mathbf{1}}(\varepsilon, \mathcal{L}(\mathcal{K}_f))$ and for all $T < \infty$ there is a constant $C_T < \infty$ such that for all $t \in [-T, T]$

$$\left\| \exp(i\widehat{\mathbf{h}}t/\varepsilon)\widehat{\mathbf{a}} \exp(-i\widehat{\mathbf{h}}t/\varepsilon) - \widehat{\mathbf{a}(t)} \right\| \leq \varepsilon^2 C_T. \tag{2.41}$$

with $\widehat{\mathbf{a}} := \widehat{\mathbf{a}}(0)$.

Proof. Since the right hand side of (2.38) is smooth and bounded together with its derivatives, the same holds true for its solution flow $\Phi_r^{t,\varepsilon}$ (uniformly for $t \in [-T, T]$), in particular $\widehat{\mathbf{a}(t)}$ is well-defined. It also follows that $\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{a}(t) = 2 \int_{S^2} \mathrm{d}\lambda(n) \frac{\mathrm{d}}{\mathrm{d}t} \left(a \circ \Phi_\varepsilon^t\right) \mathbf{\Delta}(n)$ is smooth and bounded together with its derivatives and that

$$\frac{\mathrm{d}}{\mathrm{d}t}\widehat{\mathbf{a}(t)} = \widehat{\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{a}(t)}.$$

Furthermore (for $\varepsilon \neq 0$) an application of the Gronwall lemma shows that

$$\frac{1}{\varepsilon}\left(\mathbf{a}(t) - \mathbf{a}_0(t)\right) \in S^1(\mathcal{L}(\mathbb{C}^2))$$

uniformly in ε and $t \in [-T, T]$ where

$$\mathbf{a}_0(t) := 2 \int_{S^2} d\lambda(n) a \circ \Phi_0^t(\cdot, \cdot, n) \mathbf{\Delta}(n).$$

Now we turn to prove (2.41). We have

$$\begin{aligned}
&\exp(i\widehat{\mathbf{h}}t/\varepsilon)\widehat{\mathbf{a}} \exp(-i\widehat{\mathbf{h}}t/\varepsilon) - \widehat{\mathbf{a}(t)} \\
&= \int_0^t \mathrm{d}s \frac{\mathrm{d}}{\mathrm{d}s} \left(\exp(i\widehat{\mathbf{h}}\frac{s}{\varepsilon}) \widehat{\mathbf{a}(t-s)} \exp(-i\widehat{\mathbf{h}}\frac{s}{\varepsilon}) \right) \\
&= \int_0^t \mathrm{d}s \exp(i\widehat{\mathbf{h}}\frac{s}{\varepsilon}) \left(\frac{i}{\varepsilon} \left(\widehat{\mathbf{h}}\widehat{\mathbf{a}(t-s)} - \widehat{\mathbf{a}(t-s)}\widehat{\mathbf{h}} \right) - \frac{\mathrm{d}}{\mathrm{d}t}\widehat{\mathbf{a}(t-s)} \right) \exp(-i\widehat{\mathbf{h}}\frac{s}{\varepsilon}).
\end{aligned}$$

It remains to show that

$$\frac{i}{\varepsilon}\left(\mathbf{h}\sharp\mathbf{a}(t)-\mathbf{a}(t)\sharp\mathbf{h}\right)=2\int_{S^2}\mathrm{d}n\left(\{h^\varepsilon,a(t)\}_{\mathbb{R}^6}+\frac{1}{\varepsilon}\{h^\varepsilon,a(t)\}_{S^2}\right)\mathbf{\Delta}(n)+\mathcal{O}(\varepsilon^2).$$

Since the right hand side equals $\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{a}(t)$ by construction, (2.41) then follows immediately by quantization.

Clearly h_0 is independent of n. We also know that $a_0(t)$ is independent of n since a is independent of n and Φ^t_{0q},Φ^t_{0p} depend only on q,p by construction. Therefore we have

$$\begin{aligned}
&\frac{i}{\varepsilon}\left(\mathbf{h}\sharp\mathbf{a}(t)-\mathbf{a}(t)\sharp\mathbf{h}\right)\\
&= 4\int_{S^2}\mathrm{d}n\int_{S^2}\mathrm{d}m\{h_0+\varepsilon\sqrt{3}\Omega\cdot m,a_0(t)\}_{\mathbb{R}^6}\mathbf{\Delta}(m)\mathbf{\Delta}(n)\\
&\quad +4\int_{S^2}\mathrm{d}n\int_{S^2}\mathrm{d}m\{h_0,a(t)-a_0(t)\}_{\mathbb{R}^6}\mathbf{\Delta}(m)\mathbf{\Delta}(n)\\
&\quad +i[\mathbf{h}_1,\mathbf{a}(t)]\\
&= 2\int_{S^2}\mathrm{d}n\{h^\varepsilon,a(t)\}_{\mathbb{R}^6}\mathbf{\Delta}(n)+\mathcal{O}(\varepsilon^2)\\
&\quad +i[\frac{1}{2}\Omega\cdot\boldsymbol{\sigma},\mathbf{a}(t)]
\end{aligned}$$

where the term $\{\varepsilon\sqrt{3}\Omega\cdot m,a(t)-a_0(t)\}_{\mathbb{R}^6}$ has been dropped because $a(t)-a_0(t)=\mathcal{O}(\varepsilon)$. It remains to show that $\frac{i}{2}[\Omega\cdot\boldsymbol{\sigma},\mathbf{a}(t)]=2\int_{S^2}\mathrm{d}n\frac{1}{\varepsilon}\{h^\varepsilon,a(t)\}_{S^2}\mathbf{\Delta}(n)$. This becomes clear by

$$\begin{aligned}
&\frac{i}{2}[\Omega\cdot\boldsymbol{\sigma},\mathbf{a}_\varepsilon(t)]\\
&= i\int_{S^2}\mathrm{d}n a\circ\Phi^{t,\varepsilon}_r(\cdot,\cdot,n)\,[\Omega\cdot\boldsymbol{\sigma},\mathbf{\Delta}(n)]\\
&= \sqrt{3}\int_{S^2}\mathrm{d}n a\circ\Phi^{t,\varepsilon}_r(\cdot,\cdot,n)\,(\Omega\times n)\cdot\boldsymbol{\sigma}\\
&= 2\int_{S^2}\mathrm{d}n a\circ\Phi^{t,\varepsilon}_r(\cdot,\cdot,n)\,(\Omega\times n)\cdot\nabla_n\mathbf{\Delta}(n)\\
&= 2\int_{S^2}\mathrm{d}n\nabla_n\left(a\circ\Phi^{t,\varepsilon}_r(\cdot,\cdot,n)\right)(\Omega\times n)\,\mathbf{\Delta}(n)\\
&= \frac{2}{\varepsilon}\int_{S^2}\mathrm{d}n\{h^\varepsilon,a(t)\}_{S^2}\mathbf{\Delta}(n)
\end{aligned}$$

where we used that $\nabla_n(\Omega\times n)=0$ for the integration by parts. ■

If we reduce the desired order to $\mathcal{O}(\varepsilon)$, we can deal with arbitrary observables.

Proposition 2.18 *Let $\Phi_r^{t,0}$ be the solution flow of (2.38) for $\varepsilon = 0$ and $a \in C_b^\infty(\mathbb{R}^6 \times S^2, \mathbb{C})$. Then for all $T < \infty$ there is a constant $C_T < \infty$ such that for all $t \in [-T, T]$*

$$\left\| \exp(i\widehat{\mathbf{h}}t/\varepsilon)\widehat{a}\exp(-i\widehat{\mathbf{h}}t/\varepsilon) - \widehat{a \circ \Phi_r^{t,0}} \right\| \leq \varepsilon C_T. \tag{2.42}$$

Proof. As in the proof of proposition 2.17 it is enough to show that

$$\frac{i}{\varepsilon}\left(\mathbf{h}\sharp\mathbf{a}(t) - \mathbf{a}(t)\sharp\mathbf{h}\right) = 2\int_{S^2} \mathrm{d}n \left(\{h, a(t)\}_{\mathbb{R}^6} + \frac{1}{\varepsilon}\{h, a(t)\}_{S^2} \right) \mathbf{\Delta}(n) + \mathcal{O}(\varepsilon).$$

Note that in contrast to proposition 2.17 a does now depend on n in general. Therefore we have

$$\begin{aligned}
&\frac{i}{\varepsilon}\left(\mathbf{h}\sharp\mathbf{a}(t) - \mathbf{a}(t)\sharp\mathbf{h}\right) \\
&= 4\int_{S^2} \mathrm{d}n \int_{S^2} \mathrm{d}m \{h_0, a(t)\}_{\mathbb{R}^6} \mathbf{\Delta}(m)\mathbf{\Delta}(n) + i[\mathbf{h}_1, \mathbf{a}(t)] + \mathcal{O}(\varepsilon) \\
&= 2\int_{S^2} \mathrm{d}n \{h_0, a(t)\}_{\mathbb{R}^6} \mathbf{\Delta}(n) + i[\frac{1}{2}\Omega \cdot \boldsymbol{\sigma}, \mathbf{a}(t)] + \mathcal{O}(\varepsilon) \\
&= 2\int_{S^2} \mathrm{d}n \{h_0, a(t)\}_{\mathbb{R}^6} \mathbf{\Delta}(n) + \frac{2}{\varepsilon}\int_{S^2} \mathrm{d}n \{h^\varepsilon, a(t)\}_{S^2} \mathbf{\Delta}(n) + \mathcal{O}(\varepsilon).
\end{aligned}$$

and (2.42) follows as in proposition 2.17. ■

2.3.2 Translation to the Zak representation

Propositions 2.17 and 2.18 approximate the time evolution of the quantization of a symbol $\widehat{\mathbf{a}}$ in reference space, i.e. the quantity

$$\exp(i\widehat{\mathbf{h}}t/\varepsilon)\widehat{\mathbf{a}}\exp(-i\widehat{\mathbf{h}}t/\varepsilon). \tag{2.43}$$

However, if we want to describe the time evolution of a observable $B \in \mathcal{L}(L^2(\mathbb{R}^3) \otimes \mathbb{C}^4)$ in the Zak representation, i.e. the quantity

$$\exp(iH_Z^\varepsilon t/\varepsilon) B \exp(-iH_Z^\varepsilon t/\varepsilon), \tag{2.44}$$

we have to relate (2.43) and (2.44) using theorem 2.6. Therefore it follows immediately that B must have the form

$$\begin{aligned}
B &= U^{\varepsilon *}\left(\widehat{\mathbf{a}} \oplus \mathbf{0}\right) U^\varepsilon \qquad (2.45)\\
&= \mathcal{W}(u^* \sharp (\mathbf{a} \oplus \mathbf{0}) \sharp u) + \mathcal{O}(\varepsilon^\infty) \\
&= : \widehat{\mathbf{b}} + \mathcal{O}(\varepsilon^\infty)
\end{aligned}$$

where $\mathbf{a}$ satisfies the conditions of propositions 2.17 or 2.18 in order to allow for a semiclassical limit. In this case we have

$$\begin{aligned}&\exp(iH_Z^\varepsilon t/\varepsilon)\widehat{\mathbf{b}}\exp(-iH_Z^\varepsilon t/\varepsilon) \\ =\;& U^{\varepsilon *}\left(\exp(-i\widehat{h}t)\widehat{\mathbf{a}}\exp(-i\widehat{h}t)\oplus\mathbf{0}\right)U^\varepsilon+\mathcal{O}(\varepsilon^\infty(1+|t|)) \\ =\;& \mathcal{W}(u^*\sharp\mathbf{a}(t)\sharp u)+\mathcal{O}(\varepsilon^\infty(1+|t|)).\end{aligned} \tag{2.46}$$

In the case of proposition 2.18 we have the following result:

Proposition 2.19 *Let* $b\in C_b^\infty(\mathbb{R}^6\times S^2,\mathbb{C})$ *and* $\mathbf{b}\in S^{\mathbf{1}}(\mathbb{R}^6,\mathcal{L}(\mathcal{H}_f))$ *be given by*

$$\mathbf{b}:=2\int_{S^2}d\lambda(n)b(\cdot,\cdot,n)\tilde{\mathbf{\Delta}}(\cdot,\cdot,n)$$

with

$$\tilde{\mathbf{\Delta}}(q,p,n)=u^*\sharp\left(\mathbf{\Delta}(n)\oplus\mathbf{0}\right)\sharp u. \tag{2.47}$$

Then we have

$$\exp(iH_Z^\varepsilon t/\varepsilon)\widehat{\mathbf{b}}\exp(-iH_Z^\varepsilon t/\varepsilon)-\mathcal{W}(2\int_{S^2}d\lambda(n)b\circ\Phi_r^{t,0}(\cdot,\cdot,n)\tilde{\mathbf{\Delta}}(q,p,n))=\mathcal{O}(\varepsilon)$$

uniformly for any finite time interval.

Proof. We have

$$\begin{aligned}&u^*\sharp\mathbf{a}(t)\sharp u \\ =\;& u_0^*2\int_{S^2}\mathrm{d}\lambda(n)a\circ\Phi_r^{t,0}(\cdot,\cdot,n)u_0u^*\sharp\mathbf{\Delta}(n)\sharp u+\mathcal{O}(\varepsilon) \\ =\;& 2\int_{S^2}\mathrm{d}\lambda(n)a\circ\Phi_r^{t,0}(\cdot,\cdot,n)u^*\sharp\mathbf{\Delta}(n)\sharp u+\mathcal{O}(\varepsilon)\end{aligned}$$

because $a\circ\Phi_r^{t,0}(\cdot,\cdot,n)$ is scalar-valued. Now the statement follows immediately with (2.45). ∎

In the case of proposition 2.17 the following lemma allows us to incorporate the Weyl product with u and u^* into the flow.

Lemma 2.20 *Let* $\mathbf{a}\in S^{\mathbf{1}}(\varepsilon,\mathcal{L}(\mathcal{K}_f))$ *with* a_0 *independent of* n *and*

$$\mathbf{b}:=u^*\sharp\left(\mathbf{a}\oplus\mathbf{0}\right)\sharp u.$$

Then

$$\mathbf{a} = 2\int_{S^2} d\lambda(n)\,(b\circ T_+)\,(\cdot,\cdot,n)\boldsymbol{\Delta}(n) + \mathcal{O}(\varepsilon^2) \tag{2.48}$$

and vice versa

$$\mathbf{b} =2\int_{S^2} d\lambda(n)\,(a\circ T_-)\,(\cdot,\cdot,n)\tilde{\boldsymbol{\Delta}}(q,p,n) + \mathcal{O}(\varepsilon^2) \tag{2.49}$$

with

$$T_\pm(q,p,n) = (q \pm \varepsilon\,(\nabla A)^\top \mathcal{A}(q-A(p),n), p \pm \varepsilon\mathcal{A}(q-A(p),n),n)$$

and

$$b(q,p,n) := Tr(\mathbf{b}(q,p)\tilde{\boldsymbol{\Delta}}(q,p,n)).$$

Proof. We prove (2.48). Then (2.49) follows by Moyal-multiplying with u^* and u and observing that T_- inverts T_+ up to order $\mathcal{O}(\varepsilon^2)$ as can be seen by Taylor-expanding $T_-\circ T_+$ and neglecting terms of order $\mathcal{O}(\varepsilon^2)$. As in proposition 2.19

$$\begin{aligned}\mathbf{a}_0 \oplus \mathbf{0} &= 2\int_{S^2} \mathrm{d}\lambda(n) a_0 \boldsymbol{\Delta}(n)\\ &= 2\int_{S^2} \mathrm{d}\lambda(n) b_0 \boldsymbol{\Delta}(n)\end{aligned}$$

agrees with the principal symbol of $2\int_{S^2}\mathrm{d}\lambda(n)\,(b\circ T_+)\,(\cdot,\cdot,n)\boldsymbol{\Delta}(n)$ because $T_+(\tilde{q},p,n) = (\tilde{q},p,n) + \mathcal{O}(\varepsilon)$. In particular we have $a_0 = b_0$. To compute the subprincipal symbol $\mathbf{a}_1$ in terms of $\mathbf{b}$ one proceeds as in the proof of corollary 2.8. We have

$$(\mathbf{a}\oplus\mathbf{0})\,\sharp u = u\sharp b$$

and therefore

$$\mathbf{a}_1\oplus\mathbf{0} = \left(u_0\mathbf{b}_1 + (u_0\sharp\mathbf{b}_0)_1 - ((\mathbf{a}_0\oplus\mathbf{0})\,\sharp u_0)_1 + u_1\mathbf{b}_0 - (\mathbf{a}_0\oplus\mathbf{0})\,u_1\right)u_0^*.$$

Projecting from both sides with π_r doesn't change the left hand side, but on the right hand side the last two terms cancel each other because $\mathbf{b}_0 = b_0\pi_0$ and $\mathbf{a}_0 = a_0\mathbf{1}$. For the same reason we can replace $\mathbf{b}_0$ by $b_0\mathbf{1}$ and $\mathbf{a}_0$ by $a_0\mathbf{1}$ and arrive at

$$\begin{aligned}\mathbf{a}_1\oplus\mathbf{0} &= u_0\mathbf{b}_1u_0^* - \frac{i}{2}\pi_r\{u_0,b_0\mathbf{1}\}u_0^*\pi_r + \frac{i}{2}\{\pi_r a_0,u_0\}u_0^*\pi_r\\ &= u_0\mathbf{b}_1u_0^* + i\pi_r\{b_0\mathbf{1},u_0\}u_0^*\pi_r\\ &= u_0\mathbf{b}_1u_0^* - i\nabla_q b_0\pi_r\cdot\left(\nabla U^{\mathrm{per}}\circ\widetilde{q}\right)\nabla A u_0^*\pi_r\\ &\quad -i\nabla_p b_0\pi_r\cdot\left(\nabla U^{\mathrm{per}}\circ\widetilde{q}\right)u_0^*\pi_r\\ &= u_0\mathbf{b}_1u_0^* + \nabla_q b_0\pi_r\cdot(\nabla A)^\top\mathcal{A}\circ\widetilde{q} + \nabla_p b_0\mathbf{1}\cdot\mathcal{A}\circ\widetilde{q}\end{aligned}$$

with

$$\mathcal{A}_{\nu,\mu}(k) = i \left\langle \psi_n(k), \nabla_k \psi_m(k) \right\rangle_{\mathcal{H}_f}, \quad \nu, \mu = 1, 2$$

as in corollary 2.8. Writing the last line as an integral over S^2 and using that $u_0 \mathbf{b}_1 u_0^* = u\sharp\mathbf{b}_1\sharp u^* + \mathcal{O}(\varepsilon)$ we have

$$\begin{aligned} \mathbf{a}_1 \oplus \mathbf{0} &= 2\int_{S^2} \mathrm{d}\lambda(n) b_1(\cdot,\cdot,n)\mathbf{\Delta}(n) \\ &\quad +2\int_{S^2} \mathrm{d}\lambda(n)\nabla_q b_0 \cdot (\nabla A)^\top \mathcal{A}(\widetilde{q},n)\mathbf{\Delta}(n) \\ &\quad +2\int_{S^2} \mathrm{d}\lambda(n)\nabla_p b_0 \cdot \mathcal{A}(\widetilde{q},n)\mathbf{\Delta}(n). \end{aligned}$$

A comparison with the Taylor expansion of $b \circ T_+$ now proves the claim. ■

We note furthermore that with $\tilde{T}_+ := F \circ T_+ \circ F^{-1}$ we have

$$\begin{aligned} &\left(F \circ T_+ \circ F^{-1}\right)(\widetilde{q}, p, n) \\ &= F \circ T_+(\widetilde{q} + A(p), p, n) \\ &= F(\widetilde{q} + A(p) + \varepsilon (\nabla A(p))^\top \mathcal{A}(\widetilde{q},n), p + \varepsilon\mathcal{A}(\widetilde{q},n), n) \\ &= (\widetilde{q} + A(p) - A(p + \varepsilon\mathcal{A}(\widetilde{q},n)) + \varepsilon (\nabla A(p))^\top \mathcal{A}(\widetilde{q},n), p + \varepsilon\mathcal{A}(\widetilde{q},n), n) \\ &= (\widetilde{q} + \varepsilon \Big((\nabla A(p))^\top - \nabla A(p)\Big) \mathcal{A}(\widetilde{q},n), p + \varepsilon\mathcal{A}(\widetilde{q},n), n) + \mathcal{O}(\varepsilon^2) \\ &= (\widetilde{q} + \varepsilon\mathcal{A}(\widetilde{q},n) \times B(p), p + \varepsilon\mathcal{A}(\widetilde{q},n), n) + \mathcal{O}(\varepsilon^2) \end{aligned} \tag{2.50}$$

and analogously for T_-. Now we can translate the flow $\Phi_r^{t,\varepsilon}$ of (2.38) into a flow $\Phi_Z^{t,\varepsilon}$ in the Zak representation.

Proof. (of theorem 2.14) By construction we have $\widehat{\mathbf{b}} = \Pi_Z^\varepsilon \widehat{\mathbf{b}} \Pi_Z^\varepsilon + \mathcal{O}(\varepsilon^\infty)$, therefore theorem 2.6 tells us that

$$\begin{aligned} &\exp(iH_Z^\varepsilon t/\varepsilon)\widehat{\mathbf{b}}\exp(-iH_Z^\varepsilon t/\varepsilon) \\ &= U^{\varepsilon *}\left(\Big(\exp(-i\widehat{h}t)\Big)\,\widehat{\mathbf{a}}\,\Big(\exp(-i\widehat{h}t)\Big) \oplus \mathbf{0}\right) U^\varepsilon + \mathcal{O}(\varepsilon^\infty) \end{aligned}$$

with $\mathbf{a} \oplus \mathbf{0} := u\sharp\mathbf{b}\sharp u^*$. Proposition 2.17 tells us that

$$\begin{aligned} &\exp(-i\widehat{h}t)\widehat{\mathbf{a}}\exp(-i\widehat{h}t) \\ &= \mathcal{W}(2\int_{S^2} \mathrm{d}\lambda(n) a \circ \Phi_r^{t,\varepsilon}(\cdot,\cdot,n)\mathbf{\Delta}(n)) + \mathcal{O}(\varepsilon^2). \end{aligned}$$

Using lemma 2.20 we have that

$$\begin{aligned} &\exp(iH_Z^\varepsilon t/\varepsilon)\widehat{\mathbf{b}}\exp(-iH_Z^\varepsilon t/\varepsilon) \\ &= \mathcal{W}(2\int_{S^2} \mathrm{d}\lambda(n) b \circ T_+ \circ \Phi_r^{t,\varepsilon} \circ T_-(\cdot,\cdot,n)\mathbf{\Delta}(n)) + \mathcal{O}(\varepsilon^2). \end{aligned}$$

It remains to show that

$$T_+ \circ \Phi_r^{t,\varepsilon} \circ T_- = \Phi_Z^{t,\varepsilon} + \mathcal{O}(\varepsilon^2)$$

resp. in terms of the kinetic momentum to show that

$$\tilde{T}_+ \circ \tilde{\Phi}_r^{t,\varepsilon} \circ \tilde{T}_- = \tilde{\Phi}_Z^{t,\varepsilon} + \mathcal{O}(\varepsilon^2)$$

where (as before) $\tilde{\Phi}_Z^{t,\varepsilon} := F \circ \Phi_Z^{t,\varepsilon} \circ F^{-1}$ etc. To do so, it is, using Gronwall's lemma, enough to show that the vector fields agree up to order $\mathcal{O}(\varepsilon^2)$. To start the computation, we recall the vector field of $\tilde{\Phi}_r^{t,\varepsilon}$ given in (2.40) as well as the explicit formula $\widetilde{T}_+(\widetilde{q}, p, n) = (\widetilde{q} + \varepsilon\mathcal{A}(\widetilde{q}, n) \times B(p), p + \varepsilon\mathcal{A}(\widetilde{q}, n), n)$. We call the physical variables $\widetilde{Q}, \Pi$ and n and start with the computation of $\dot{\widetilde{Q}}$:

$$\begin{aligned}
\dot{\widetilde{Q}}_j &= \dot{\widetilde{q}}_j + \varepsilon\frac{\mathrm{d}}{\mathrm{d}t}(\mathcal{A}(\widetilde{q}, n) \times B(p))_j \\
&= -\partial_j\phi(p) + (\dot{p} \times B(p))_j - \varepsilon\left(\partial_j\nabla\phi(p) - \nabla E(\widetilde{q}) \times \partial_j B(p)\right) \cdot \mathcal{A}(\widetilde{q}, n) \\
&\quad +\varepsilon\partial_j B(p) \cdot \mathcal{M}(\widetilde{q}, n) + \varepsilon\left(\dot{\mathcal{A}}(\widetilde{q}, n) \times B(p)\right)_j + \varepsilon\left(\mathcal{A}(\widetilde{q}, n) \times \dot{B}(p)\right)_j \\
&= -\partial_j\phi(p) - \varepsilon\nabla\partial_j\phi(p) \cdot \mathcal{A}(\widetilde{q}, n) + \varepsilon\partial_j B(p) \cdot \mathcal{M}(\widetilde{q}, n) \\
&\quad + (\dot{p} \times B(p))_j + \varepsilon\left(\dot{\mathcal{A}}(\widetilde{q}, n) \times B(p)\right)_j \\
&\quad +\varepsilon\nabla E(\widetilde{q}) \times \partial_j B(p) \cdot \mathcal{A}(\widetilde{q}, n) + \varepsilon\left(\mathcal{A}(\widetilde{q}, n) \times \dot{B}(p)\right)_j + \mathcal{O}(\varepsilon^2) \\
&= -\partial_j\phi(\Pi) + \varepsilon\partial_j B(\Pi) \cdot \mathcal{M}(\widetilde{Q}, n) + \left(\dot{\Pi} \times B(p)\right)_j \\
&\quad +\varepsilon\dot{\Pi} \times \partial_j B(\Pi) \cdot \mathcal{A}(\widetilde{Q}, n) + \varepsilon\left(\mathcal{A}(\widetilde{Q}, n) \times \dot{B}(\Pi)\right)_j + \mathcal{O}(\varepsilon^2) \\
&= -\partial_j\phi(\Pi) + \varepsilon\partial_j B(\Pi) \cdot \mathcal{M}(\widetilde{Q}, n) + \left(\dot{\Pi} \times B(\Pi)\right)_j + \mathcal{O}(\varepsilon^2)
\end{aligned}$$

In the third equality we just regrouped the terms to make the following changes in the fourth equality more transparent. Then we used Taylor expansions and the fact that in first order terms we can exchange the arguments $\widetilde{q}, p$ by $\widetilde{Q}, \Pi$ as well as $\nabla E(\widetilde{q})$ by $\dot{\Pi}$. The final equality becomes now clear by noticing that

$$\begin{aligned}
&\varepsilon\dot{\Pi} \times \partial_j B(\Pi) \cdot \mathcal{A}(\widetilde{Q}, n) + \varepsilon \left(\mathcal{A}(\widetilde{Q}, n) \times \dot{B}(\Pi)\right)_j \\
&= \varepsilon \sum_{k,l,m} e_{klm} \dot{\Pi}_l \partial_j B_m(\Pi) \mathcal{A}_k(\widetilde{Q}, n) + \varepsilon \sum_{k,m} e_{jkm} \mathcal{A}_k(\widetilde{Q}, n) \dot{B}_m(\Pi) \\
&= \varepsilon \sum_{k,l,m} \left(e_{klm} \partial_j B_m(\Pi) + e_{jkm} \partial_l B_m(\Pi)\right) \dot{\Pi}_l \mathcal{A}_k(\widetilde{Q}, n) \\
&= \varepsilon \sum_{k,l,m} \left(e_{jlm} \partial_k B_m(\Pi)\right) \dot{\Pi}_l \mathcal{A}_k(\widetilde{Q}, n) \\
&= \left(\dot{\Pi} \times (B(\Pi) - B(p))\right)_j + \mathcal{O}(\varepsilon^2)
\end{aligned}$$

where e_{klm} is the Levi-Civitä symbol. We go on with calculating $\dot{\Pi}_j$:

$$\begin{aligned}
\dot{\Pi}_j &= \dot{p}_j + \varepsilon \dot{\mathcal{A}}_j(\widetilde{q}, n) \\
&= \partial_j E(\widetilde{q}) - \varepsilon \partial_{k_j} \left(F_{\mathrm{Lor}}(\widetilde{q}, p) \cdot \mathcal{A}(\widetilde{q}, n) + B(p) \cdot \mathcal{M}(\widetilde{q}, n)\right) \\
&\quad + \varepsilon \partial_{k_l} \mathcal{A}_j(\widetilde{q}, n) \dot{\widetilde{q}}_l + \varepsilon \partial_{n_l} \mathcal{A}_j(\widetilde{q}, n) \dot{n}_l \\
&= \partial_j E(\widetilde{q}) - \varepsilon \left(\partial_{k_j} F_{\mathrm{Lor}}(\widetilde{q}, p) \cdot \mathcal{A}(\widetilde{q}, n) + B(p) \cdot \partial_{k_j} \mathcal{M}(\widetilde{q}, n)\right) \\
&\quad + \varepsilon \left(\partial_{k_l} \mathcal{A}_j(\widetilde{q}, n) - \partial_{k_j} \mathcal{A}_l(\widetilde{q}, n)\right) \dot{\widetilde{q}}_l + \varepsilon \partial_{n_l} \mathcal{A}_j(\widetilde{q}, n) \dot{n}_l \\
&= \partial_j E(\widetilde{Q}) - \varepsilon B(\Pi) \cdot \partial_{k_j} \mathcal{M}(\widetilde{Q}, n) + \varepsilon \left(\Omega_{\mathcal{A}}(\widetilde{Q}, n) \times \dot{\widetilde{Q}}\right)_j + \varepsilon \partial_{n_l} \mathcal{A}_j(\widetilde{q}, n) \dot{n}_l
\end{aligned}$$

where we used that $\dot{\widetilde{q}} = F_{\mathrm{Lor}}(\widetilde{q}, p) + \mathcal{O}(\varepsilon)$ and

$$\begin{aligned}
&\varepsilon \partial_{\widetilde{q}_j} F_{\mathrm{Lor}}(\widetilde{q}, p) \cdot \mathcal{A}(\widetilde{q}, n) \\
&= \varepsilon \nabla \partial_j E(\widetilde{q}) \times B(p) \cdot \mathcal{A}(\widetilde{q}, n) \\
&= \varepsilon B(p) \times \mathcal{A}(\widetilde{q}, n) \cdot \nabla \partial_j E(\widetilde{q}) \\
&= \partial_j E(\widetilde{q}) - \partial_j E(\widetilde{Q}) + \mathcal{O}(\varepsilon^2).
\end{aligned}$$

Observe that from the proof of proposition 2.17 it follows that we could have added an arbitrary term of order $\mathcal{O}(\varepsilon)$ to $\dot{n} = n \times \tilde{\Omega}(\widetilde{q}, p)$ in (2.40) without changing the validity of the semiclassical approximation. Therefore, for n we only have to compute the first order, i.e. we have

$$\dot{n} = n \times \tilde{\Omega}(\widetilde{Q}, \Pi).$$

■

3 Pauli-Bloch electrons

In chapter 2 we set $c = 1$ in the definition of H^ε in 2.1. The c-dependent Hamiltonian $H^{\varepsilon,c}$ reads explicitly

$$H^{\varepsilon,c} := c^2\boldsymbol{\beta} + c(-i\nabla_x - A(\varepsilon x)) \cdot \boldsymbol{\alpha} + V_\Gamma(x) + \phi(\varepsilon x). \tag{3.1}$$

The nonrelativistic limit of (3.1), i.e. the behavior of $H^{\varepsilon,c}$as c tends to infinity, has been intensively studied since the famous paper [FoWo] of Foldy and Wouthuysen. They showed in a formal calculation that $(H^{\varepsilon,c} - c^2)$ is, up to higher orders in $\frac{1}{c}$ unitarily related to the so-called Pauli Hamiltonian

$$H^{\varepsilon,P} := H^{\varepsilon,S} \otimes \mathbf{1}_{\mathbb{C}^2} - \frac{1}{2}\varepsilon B(\varepsilon x) \otimes \boldsymbol{\sigma} \tag{3.2}$$

with the usual nonrelativistic Schrödinger Hamiltonian

$$H^{\varepsilon,S} := \frac{1}{2}(-i\nabla_x - A(\varepsilon x))^2 + V_\Gamma(x) + \phi(\varepsilon x).$$

$H^{\varepsilon,P}$ is self-adjoint on $H^2(\mathbb{R}^3) \otimes \mathbb{C}^2 \subset L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$ under assumption $(A1)$.

In this chapter, we first study in section 3.1 how to relate the time evolution generated by (3.1) and the one generated by (3.2). Next, we will undertake for $H^{\varepsilon,P}$ the same program as in chapter 2 for $H^{\varepsilon,c}$: we will identify subspaces that are invariant under the dynamics generated by the unperturbed Hamiltonian, i.e. by $H^{\varepsilon=0}$ in section 3.2 by studying the unitarily transformed Hamiltonian

$$H^P_{\text{per}} := (\mathcal{U} \otimes \mathbf{1}_{\mathbb{C}^2})\, H^{\varepsilon=0,P} \left(\mathcal{U}^{-1} \otimes \mathbf{1}_{\mathbb{C}^2}\right)$$

acting on $\mathcal{H}_\tau = \mathcal{U}\left(L^2(\mathbb{R}^3)\right) \otimes \mathbb{C}^2$. In section 3.3 we will perform the space-adiabatic perturbation theory for $H^{\varepsilon,P}$ and finally, in section 3.4 we will study the semiclassical limit. Since the program is analogous to chapter 2 we will state the relevant theorems, but instead of full proofs merely comment the changes. We also note that $H^{\varepsilon,S}$ is just the nonrelativistic Schrödinger-Bloch Hamiltonian studied in [Teu], chapter 5. Clearly, all the following results for $H^{\varepsilon,P}$ differ mainly from the results derived there by an additional $\otimes\mathbf{1}_{\mathbb{C}^2}$ at the end of symbols and operators and the fact that we have an additional subprincipal term coming from $-\frac{1}{2}\varepsilon B(\varepsilon x) \otimes \boldsymbol{\sigma}$.

Remark 3.1 *For sake of notational simplicity, we suppress the superscript P for Pauli in in $H^{\varepsilon,P}$ and in all derived quantities π, u, h etc. in sections 3.2, 3.3 and 3.4. For the comparison of the Dirac and Pauli quantities, we will re-introduce the superscript in chapter* 4.

3.1 The nonrelativistic limit

As mentioned in the introduction, we first aim to compare the time evolution generated by the full Dirac Hamiltonian $H^{\varepsilon,c}$ and the one of the Pauli Hamiltonian $H^{\varepsilon,P}$. The basic ingredient is the fact, as written in [Th], cor. 6.5, that the resolvent of $H^{\varepsilon,c} - c^2$, i.e. $(H^{\varepsilon,c} - c^2 - \zeta)^{-1}$ has for each fixed $\zeta \in \mathbb{C} \setminus \mathbb{R}$ and each fixed ε a power series expansion in $\frac{1}{c}$ that is absolutely convergent in $\|\cdot\|_{\mathcal{L}(L^2)}$. A careful analysis of the proof in Thaller in our context shows that the power series converges even in $\sup_{\varepsilon\in[0,\varepsilon_0)} \|\cdot\|_{\mathcal{L}(L^2,H^1)}$ as will be important for the following.

Lemma 3.2 $(H^{\varepsilon,c}-c^2-\zeta)^{-1}$ *has, for each fixed $\zeta \in \mathbb{C} \setminus \mathbb{R}$ a power series expansion*

$$(H^{\varepsilon,c} - c^2 - \zeta)^{-1} = \sum_{n=0}^{\infty} \frac{1}{c^n} R_n^\varepsilon(\zeta)$$

that converges absolutely in $\sup_{\varepsilon\in[0,\varepsilon_0)} \|\cdot\|_{\mathcal{L}(L^2,H^1)}$ for c large (depending on ζ) enough. The first two terms are

$$\begin{aligned} R_0^\varepsilon(\zeta) &= \left(\frac{1}{2}Q^2 + V_\Gamma + \phi - \zeta\right)^{-1} P_+ \\ R_1^\varepsilon(\zeta) &= \frac{1}{2}P_+ \left(\frac{1}{2}Q^2 + V_\Gamma + \phi - \zeta\right)^{-1} Q + \frac{1}{2}Q \left(\frac{1}{2}Q^2 + V_\Gamma + \phi - \zeta\right)^{-1} P_+ \end{aligned}$$

with

$$Q = (-i\nabla_x - A(\varepsilon x)) \cdot \boldsymbol{\alpha}.$$

Proof. In [Th] it is shown that

$$\begin{aligned} &(H^{\varepsilon,c} - c^2 - \zeta)^{-1} \\ &= \left(P_+ + \frac{1}{2c^2}(cQ + \zeta)\right) K(c^{-2}) \left(\mathbf{1} + \frac{1}{2c^2}(V_\Gamma + \phi)(cQ + \zeta)K(c^{-2})\right)^{-1} \end{aligned}$$

with

$$K(c^{-2}) = \left(\mathbf{1} - \frac{1}{2c^2}\zeta^2 R_\infty^\varepsilon(\zeta)\right)^{-1} R_\infty^\varepsilon(\zeta)$$

and

$$R_\infty^\varepsilon(\zeta) = (H^{\varepsilon,\infty} - \zeta)^{-1} = \left(\frac{1}{2}Q^2 + (V_\Gamma + \phi)\, P_+ - \zeta\right)^{-1}$$

whenever all quantities are well-defined. For fixed ε, we know that

$$\|R_\infty^\varepsilon(\zeta)\|_{\mathcal{L}(L^2,H^2)} < \infty,$$

therefore one can expand $K(c^{-2})$ into a power series in $\frac{1}{c}$ that converges in $\|\cdot\|_{\mathcal{L}(L^2,H^2)}$. It follows that also $(H^{\varepsilon,c} - c^2 - \zeta)^{-1}$ can be expanded into a power series that converges in $\|\cdot\|_{\mathcal{L}(L^2,H^1)}$ (observe that $\|Q\|_{\mathcal{L}(H^2,H^1)} < \infty$). It remains to show that the expansion is uniform in ε. Since we know that $\sup_{\varepsilon\in[0,\varepsilon_0)} \|Q\|_{\mathcal{L}(H^2,H^1)} < \infty$ (because A is bounded together with its derivatives), it only remains to show that

$$\sup_{\varepsilon\in[0,\varepsilon_0)} \|R_\infty^\varepsilon(\zeta)\|_{\mathcal{L}(L^2,H^2)} < \infty.$$

To this end note that with a variant of the resolvent equation we have

$$R_\infty^\varepsilon(\zeta) = \left(\frac{1}{2}\Delta_x - \zeta\right)^{-1} \left(\mathbf{1} + (H^{\varepsilon,\infty} - \frac{1}{2}\Delta_x) R_\infty^\varepsilon\right)$$

with $\left(\frac{1}{2}\Delta_x - \zeta\right)^{-1} \in \mathcal{L}(L^2, H^2)$. Furthermore

$$(H^{\varepsilon,\infty} - \frac{1}{2}\Delta_x) = 2A(\varepsilon x)\cdot\nabla_x + \varepsilon(\nabla A)(\varepsilon x) + A(\varepsilon x)^2 + \varepsilon B(\varepsilon x) + V_\Gamma(x) + \phi(\varepsilon x),$$

i.e. $(H^{\varepsilon,\infty} - \frac{1}{2}\Delta_x)$ is bounded from H^1 to L^2 uniformly in ε (recall that V_Γ is infinitesimally bounded w.r.t. ∇_x) and we have that

$$\sup_{\varepsilon\in[0,\varepsilon_0)} \|R_\infty^\varepsilon(\zeta)\|_{\mathcal{L}(L^2,H^2)} \le C \sup_{\varepsilon\in[0,\varepsilon_0)} \|R_\infty^\varepsilon(\zeta)\|_{\mathcal{L}(L^2,H^1)}\,.$$

Since we also know that $\left(\frac{1}{2}\Delta_x - \zeta\right)^{-1} \in \mathcal{L}(H^{-1}, H^1)$ and that $(H^{\varepsilon,\infty} - \frac{1}{2}\Delta_x)$ is bounded from L^2 to H^{-1} uniformly in ε, we can repeat the argument and have

$$\sup_{\varepsilon\in[0,\varepsilon_0)} \|R_\infty^\varepsilon(\zeta)\|_{\mathcal{L}(L^2,H^1)} \le C' \sup_{\varepsilon\in[0,\varepsilon_0)} \|R_\infty^\varepsilon(\zeta)\|_{\mathcal{L}(L^2)}$$

and the result follows. ■

As explained in chapter 2, we are interested in time scales of order $\mathcal{O}(\frac{1}{\varepsilon})$. However, the difference in the time evolution between $H^{\varepsilon,c}$ and $H^{\varepsilon,P}$ comes not only from the ε-dependent external potentials, but also from the presence of the periodic potential V_Γ and therefore one cannot expect that the Pauli approximation holds over time scales of order $\mathcal{O}(\frac{1}{\varepsilon})$. Instead we study time scales of order $\mathcal{O}(c)$ and get the following result:

Proposition 3.3 *One has*

$$\big(\exp(ict(H^{\varepsilon,c}-c^2)) - \exp(ictH^{\varepsilon}_P)\otimes \mathbf{0}\big)\,\chi_{[-a,a]}(H^{\varepsilon,P})\otimes \mathbf{1} = \mathcal{O}(\frac{1}{c}(1+|t|)(a^2+1))$$

for any spectral projection $\chi_{[-a,a]}(H^{\varepsilon,P})$ *of the Pauli Hamiltonian.*

Proof. We write

$$\begin{aligned}
&\big(\exp(ictH^{\varepsilon,P})\otimes\mathbf{0} - \exp(ict(H^{\varepsilon,c}-c^2)\big)\,\big((H^{\varepsilon,P}-i)^{-1}\otimes\mathbf{0}\big)\\
&= (H^{\varepsilon,c}-c^2-i)^{-1}(\mathbf{1}+\frac{1}{2c}Q)\exp(-ictH^{\varepsilon,P})\otimes\mathbf{0}\\
&\quad -\exp(-itc(H^{\varepsilon,c}-c^2))(H^{\varepsilon,c}-c^2-i)^{-1}(\mathbf{1}+\frac{1}{2c}Q)+\mathcal{O}(\frac{1}{c})\\
&= \int_0^t \mathrm{d}s\frac{\mathrm{d}}{\mathrm{d}s}\exp(-ic(t-s)(H^{\varepsilon,c}-c^2))(H^{\varepsilon,c}-c^2-i)^{-1}\\
&\quad \times(\mathbf{1}+\frac{1}{2c}Q)\exp(-icsH^{\varepsilon,P})\otimes\mathbf{0}+\mathcal{O}(\frac{1}{c})
\end{aligned}$$

with $\mathcal{O}(\frac{1}{c})$ in the norm of bounded operators because

$$(H^{\varepsilon,c}-c^2-i)^{-1}-(H^{\varepsilon,P}-i)^{-1}=\mathcal{O}(\frac{1}{c})$$

in $\mathcal{L}(L^2,H^1)$ and $Q\in\mathcal{L}(H^1,L^2)$. Next we consider the integrand. One has

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}s}\left(\exp(-ic(t-s)(H^{\varepsilon,c}-c^2))(H^{\varepsilon,c}-c^2-i)^{-1}(\mathbf{1}+\frac{1}{2c}Q)\exp(-icsH^{\varepsilon,P})\otimes\mathbf{0}\right)\\
&= ic\exp(-ic(t-s)(H^{\varepsilon,c}-c^2))\\
&\quad\times\left((\mathbf{1}+\frac{1}{2c}Q)-(H^{\varepsilon,c}-c^2-i)^{-1}(\mathbf{1}+\frac{1}{2c}Q)\big((H^{\varepsilon,P}-i)\otimes\mathbf{0}\big)\right)\\
&\quad\times\exp(-icsH^{\varepsilon,P})\\
&= ic\exp(-ic(t-s)(H^{\varepsilon,c}-c^2))\\
&\quad\times\left((\mathbf{1}+\frac{1}{2c}Q)\big((H^{\varepsilon,P}-i)^{-1}\otimes\mathbf{1}\big)-(H^{\varepsilon,c}-c^2-i)^{-1}(\mathbf{1}+\frac{1}{2c}Q)\right)\\
&\quad\times\exp(-icsH^{\varepsilon,P})\big((H^{\varepsilon,P}-i)\otimes\mathbf{0}\big)\\
&= \mathcal{O}(\frac{1}{c})\big((H^{\varepsilon,P}-i)\otimes\mathbf{0}\big)
\end{aligned}$$

with $\mathcal{O}(\frac{1}{c})$ in the norm of bounded operators (recall that the power series of $(H^{\varepsilon,c}-c^2-i)^{-1}$ converges in $\mathcal{L}(L^2,H^1)$). Together

$$\left(\exp(-i\frac{t}{c}H^{\varepsilon,P})-\exp(-i\frac{t}{c}(H^{\varepsilon,c}-c^2))\right)\big((H^{\varepsilon,P}-i)^{-2}\otimes\mathbf{1}\big)=\mathcal{O}(\frac{1}{c})$$

in the norm of bounded operators. Now, if we project with $\chi_{[-a,a]}(H^{\varepsilon,P}) \otimes \mathbf{1}$, then

$$\begin{aligned} &\left\| \left(\exp(ict(H^{\varepsilon,c} - c^2)) - \exp(ictH^{\varepsilon,P}) \otimes \mathbf{0}\right) \left(\chi_{[-a,a]}(H^{\varepsilon,P}) \otimes \mathbf{1}\right) \right\|_{\mathcal{L}(L^2)} \\ \leq\ & \left\| \left(\exp(ict(H^{\varepsilon,c} - c^2)) - \exp(ictH^{\varepsilon,P}) \otimes \mathbf{0}\right) \left((H^{\varepsilon,P} - i)^{-2} \otimes \mathbf{1}\right) \right\|_{\mathcal{L}(L^2)} \\ & \left\| \left((H^{\varepsilon,P} - i)^{2} \otimes \mathbf{1}\right) \left(\chi_{[-a,a]}(H^{\varepsilon,P}) \otimes \mathbf{1}\right) \right\|_{\mathcal{L}(L^2)} \\ \leq\ & (a^2+1)\mathcal{O}(\frac{1}{c}). \end{aligned}$$

■

3.2 The Pauli Hamiltonian

In this section, we want to start the adiabatic analysis of (3.2) by studying the unperturbed Pauli Hamiltonian. As in section 2.1 one applies the Zak transform and has

$$(\mathcal{U} \otimes \mathbf{1}_{\mathbb{C}^2})\, H^{\varepsilon=0} \left(\mathcal{U}^{-1} \otimes \mathbf{1}_{\mathbb{C}^2}\right) = \int_{\mathbb{R}^3}^{\oplus} H_{\mathrm{per}}(k)$$

with

$$\begin{aligned} H_{\mathrm{per}}(k) &= \left(\frac{1}{2}(-i\nabla_y + k)^2 + V_\Gamma(y)\right) \otimes \mathbf{1}_{\mathbb{C}^2} \\ &=: H^S_{\mathrm{per}} \otimes \mathbf{1}_{\mathbb{C}^2}, \quad k \in \mathbb{R}^3. \end{aligned}$$

$H_{\mathrm{per}}(k)$ is self-adjoint with domain $\mathcal{D} := H^2(\mathbb{T}^3) \otimes \mathbb{C}^2 \subset L^2(\mathbb{T}^3) \otimes \mathbb{C}^2 =: \mathcal{H}_f$ for each fixed k and τ-equivariant as function of k. The same holds true for $H^S_{\mathrm{per}}(k)$ with domain $\mathcal{D}^S := H^2(\mathbb{T}^3) \subset L^2(\mathbb{T}^3) =: \mathcal{H}^S_f$. Each $H_{\mathrm{per}}(k)$ (and $H^S_{\mathrm{per}}(k)$) has purely discrete spectrum accumulating at infinity because

$$\begin{aligned} R_{\mathrm{per}}(\zeta, k) &:= (H_{\mathrm{per}}(k) - \zeta)^{-1} \\ &=: R^S_{\mathrm{per}}(\zeta, k) \otimes \mathbf{1}_{\mathbb{C}^2} \end{aligned}$$

is compact. In contrast to chapter 2, H_{per} is semibounded and therefore the labelling of the eigenvalues causes no problems. We denote the eigenvalues of $H_{\mathrm{per}}(k)$ in increasing order and according to their multiplicity with $E_n(k)$, $n \in \mathbb{N}_0$. Note that to each eigenvalue of H^S_{per} corresponds an eigenvalue of $H_{\mathrm{per}}(k)$ with twice the degree of degeneracy. This degeneracy corresponds to the symmetries of lemma 2.2 and corollary 2.3, the latter one now being valid even without inversion-symmetric V_Γ. To reflect this structure, we introduce $E^S_n(k)$ as the n-th eigenvalue of $H^S_{\mathrm{per}}(k)$ and note that with this convention we have

$$E_{2n+j} = E^S_n, \quad n \in \mathbb{N}_0, j = 0, 1.$$

Furthermore, the corresponding eigenfunctions $\varphi_n(k)$ of $H_{\text{per}}(k)$ and $\varphi_n^S(k)$ of $H_{\text{per}}^S(k)$ satisfy the relation

$$\varphi_{2n+j}(k) = \varphi_n^S(k) \otimes e_j, \quad n \in \mathbb{N}_0, j = 0, 1$$

where e_j is the j-th unit vector in $\mathbb{C}^2$. Finally we note that the resolvents $R_{\text{per}}(\zeta, k)$ and $R_{\text{per}}^S(\zeta, k)$ are smooth in k and that all its partial derivatives are holomorphic in ζ on $\{(k, \zeta) : \zeta \notin \sigma(H_{\text{per}}(k)) = \sigma(H_{\text{per}}^S(k))\}$.

3.3 Adiabatic perturbation theory

Now we want to analyze the Hamiltonian

$$\begin{aligned} H_Z^\varepsilon \quad : &= (\mathcal{U} \otimes \mathbf{1}_{\mathbb{C}^2})\, H^\varepsilon \left(\mathcal{U}^{-1} \otimes \mathbf{1}_{\mathbb{C}^2}\right) \\ &= \left(\frac{1}{2}(-i\nabla_y + k - A(\varepsilon\nabla_k^\tau))^2 + V_\Gamma(y) + \phi(\varepsilon\nabla_k^\tau)\right) \otimes \mathbf{1}_{\mathbb{C}^2} - \varepsilon B(\varepsilon\nabla_k^\tau) \otimes \boldsymbol{\sigma} \\ &=: H_Z^{\varepsilon,S} \otimes \mathbf{1}_{\mathbb{C}^2} - \varepsilon \frac{1}{2} B(\varepsilon\nabla_k^\tau) \otimes \boldsymbol{\sigma}. \end{aligned}$$

To this end, we start with the observation that H_Z^ε is the Weyl-quantization of the symbol $H_0 + \varepsilon H_1 \in S_\tau^{w^2}(\varepsilon, \mathcal{L}(\mathcal{D}, \mathcal{H}_f))$ with

$$\begin{aligned} H_0(q,p) &= \left(\frac{1}{2}(-i\nabla_y + q - A(p))^2 + V_\Gamma(y) + \phi(p)\right) \otimes \mathbf{1}_{\mathbb{C}^2} \qquad (3.3) \\ &=: H_0^S(q,p) \otimes \mathbf{1}_{\mathbb{C}^2}, \\ H_1(q,p) &= -\mathbf{1}_{L^2(\mathbb{T}^3)} \otimes \left(\frac{1}{2} B(p) \cdot \boldsymbol{\sigma}\right). \end{aligned}$$

Due to the eigenvalue structure of $H_{\text{per}}(k)$, every isolated family stems from an isolated family $\{E_n^S\}_{n \in \mathcal{I}^S}$ of $H_{\text{per}}^S(k)$. Therefore, we first fix (w.l.o.g.) an isolated family $\{E_{2n+j}(k)\}_{n \in \mathcal{I}, j=0,1}$ of bands of $H_{\text{per}}(k)$ with $\mathcal{I} = [I_-, I_+] \cap \mathbb{N}_0$ as well as enclosing circles $\Lambda_{\text{per}}(k)$. The corresponding projection satisfies

$$\begin{aligned} P_{\text{per}}(k) &= \int_{\Lambda_{\text{per}}^P(k)} \mathrm{d}\zeta\, R_{\text{per}}(\zeta, k) \\ &= P_{\text{per}}^S(k) \otimes \mathbf{1}_{\mathbb{C}^2} \qquad (3.4) \end{aligned}$$

where $P_{\text{per}}^S(k)$ corresponds to the isolated family $\{E_n(k)\}_{n \in \mathcal{I}}$ of $H_{\text{per}}^S(k)$. Following [Pa] there is a smooth, right τ-covariant unitary $U_{\text{per}}^S(k) \in \mathcal{U}(\mathcal{H}_f^S)$ intertwining $P_{\text{per}}^S(k)$ and $P_{\text{per}}^S(0) =: \pi_r^S$, i.e.

$$U_{\text{per}}^S(k)^* P_{\text{per}}^S(k) U_{\text{per}}^S(k) = P_{\text{per}}^S(0).$$

It follows that also

$$U^P_{\mathrm{per}}(k) := U^S_{\mathrm{per}}(k) \otimes \mathbf{1}_{\mathbb{C}^2} \tag{3.5}$$

is smooth, right τ-covariant and intertwines $P_{\mathrm{per}}(k)$ and $P_{\mathrm{per}}(0) =: \pi_r$. Defining $\psi_n(k) := U_{\mathrm{per}}(k)\chi_n$ with $\chi_n := \varphi_n(0)$ we have

$$P_{\mathrm{per}}(k) = \sum_{n\in\mathcal{I},j=0,1} \left\langle \psi_{2n+j}(k), \cdot \right\rangle \psi_{2n+j}(k)$$

where

$$\psi_{2n+j}(k) =: \psi^S_n(k) \otimes e_j, \quad n \in \mathcal{I}^S, j = 0, 1$$

are smooth and τ-equivariant in k, but not necessarily eigenfunctions of $H_{\mathrm{per}}(k)$. We also introduce

$$\begin{aligned} \mathcal{K}_f \;\; &: \;\; = \mathrm{Ran} P_{\mathrm{per}}(0) \\ &= \;\; \left(\mathrm{Ran} P^S_{\mathcal{I}^S}(0)\right) \otimes \mathbb{C}^2 \\ &= \;\; : \mathcal{K}^S_f \otimes \mathbb{C}^2, \end{aligned}$$

i.e. $\mathcal{K}_f \cong \mathbb{C}^{2N}$ with $2N = |\mathcal{I}|$. Now we can apply the same technique as in chapter 2 and obtain an analogous result.

Theorem 3.4 (Peierls substitution) *Let $\{E_{2n+j}(k)\}_{n\in\mathcal{I},j=0,1}$ be an isolated family of bands in the sense of Definition 2.5 and let Assumption be satisfied. Then there exist*

(i) an orthogonal projection $\Pi^\varepsilon_Z \in \mathcal{L}(\mathcal{H}_\tau)$,

(ii) a unitary map $U^\varepsilon \in \mathcal{L}(\mathcal{H}_\tau, \mathcal{H}_r)$, and

(iii) a self-adjoint operator $\widehat{\mathbf{h}} \in L^2(\mathbb{T}^{3*}, \mathcal{K}_f)$

such that

$$\|[\exp(-iH^\varepsilon_Z t), \Pi^\varepsilon_Z]\| = \mathcal{O}(\varepsilon^\infty(1 + |t|))$$

and

$$\left\|\exp(-iH^\varepsilon_Z t)\Pi^\varepsilon_Z - U^{\varepsilon *}\left(\exp(-i\widehat{\mathbf{h}}t) \oplus \mathbf{0}\right) U^\varepsilon\right\| = \mathcal{O}(\varepsilon^\infty(1 + |t|)).$$

The effective Hamiltonian $\widehat{\mathbf{h}}$ is the Weyl quantization of a semiclassical symbol $\mathbf{h} \in S^1_{\tau\equiv\mathbf{1}}(\varepsilon, \mathcal{L}(\mathcal{K}_f))$ whose asymptotic expansion in ε can be computed to any order.

Proof. The proof is exactly analogous to the proofs in chapter 2, except that one has to replace the order function w by w^2 (and one has a nonvanishing subprincipal symbol H_1). However, the new order function causes no problems regarding lemma B.3. ■

Since $H_{\mathrm{per}} = H^S_{\mathrm{per}}(q,p)\otimes\mathbf{1}_{\mathbb{C}^2}$, $P_{\mathrm{per}}(k) = P^S_{\mathrm{per}}(k)\otimes\mathbf{1}_{\mathbb{C}^2}$ and $U_{\mathrm{per}}(k) = U^S_{\mathrm{per}}(k)\otimes\mathbf{1}_{\mathbb{C}^2}$, one might ask whether also the quantities of theorem 3.4 have this form. Indeed, if we denote by $u^S, \pi^S, \mathbf{h}^S$ etc. the quantities that appear when applying space-adiabatic analysis on $H^{\varepsilon,S}_Z$, we have the following result which is useful for the explicit determination of h as well as for the following semiclassical limit.

Lemma 3.5 *We have*

$$\pi_j = \pi^S_j \otimes \mathbf{1}_{\mathbb{C}^2}, \quad j = 0, 1$$

and

$$u_j = u^S_j \otimes \mathbf{1}_{\mathbb{C}^2}, \quad j = 0, 1.$$

Proof. For $j = 0$ this follows immediately from $\pi_0(q,p) = P_{\mathrm{per}}(q - A(p))$ and $u_0(q,p) = U_{\mathrm{per}}(q - A(p))$. For π_1, we first observe that

$$\begin{aligned} R_1(\zeta) &= -\left(R_0(\zeta)\sharp(H_0-\zeta)\right)_1 R_0(\zeta) - R_0(\zeta)H_1R_0(\zeta) \\ &= -\left(\left(R^S_0(\zeta)\sharp(H^S_0-\zeta)\right)_1 R^S_0(\zeta)\right)\otimes\mathbf{1}_{\mathbb{C}^2} + \frac{1}{2}R^S_0(\zeta)R^S_0(\zeta)\otimes(B(p)\cdot\boldsymbol{\sigma}) \\ &= R^S_1(\zeta)\otimes\mathbf{1}_{\mathbb{C}^2} + \frac{1}{2}\left(R^S_0(\zeta)\right)^2\otimes(B(p)\cdot\boldsymbol{\sigma}). \end{aligned}$$

On the other hand

$$\int_\Lambda \mathrm{d}\zeta\,\left(R^S_0(\zeta)\right)^2 = \mathbf{0}$$

therefore

$$\pi_1 = \pi^S_1 \otimes \mathbf{1}_{\mathbb{C}^2}$$

follows. Since for the construction of u_1 only u_0, π_0 and π_1 are used, also

$$u_1 = u^S_1 \otimes \mathbf{1}_{\mathbb{C}^2}$$

is clear. ■

Now we can also compute the principal and (in the case of a single eigenvalue band) subprincipal symbol.

Corollary 3.6 *The principal symbol of the effective Hamiltonian in theorem (3.4) is given by*

$$\mathbf{h}_0(q,p) = \mathbf{h}^S_0(q,p)\otimes\mathbf{1}_{\mathbb{C}^2}$$

where h_0^S has matrix elements

$$\mathbf{h}_0^S(q,p)_{\nu,\mu} = \left\langle \psi_\nu^S(q-A(p)), H_0^S(q,p)\psi_\mu^S(q-A(p))\right\rangle, \quad \nu,\mu \in \{1,\dots,N\}$$

where H_0^S is defined in (3.3). If the family $\{E_n\}_{n\in\mathcal{I}}$ consist of a single 2-fold degenerate eigenvalue $E_*(k) = E_*^S(k)$, then we have (in the notation of theorem 3.4)

$$\mathbf{h}_0(q,p) = \left(E_*^S(\widetilde{q}) + \phi(p)\right)\mathbf{1}_{\mathcal{K}_f^S}\otimes \mathbf{1}_{\mathbb{C}^2}$$

and

$$\begin{aligned}\mathbf{h}_1(q,p) &= \left(-F_{Lor}^S(\widetilde{q},p)\cdot\mathcal{A}^S(\widetilde{q}) - B(p)\cdot\mathcal{M}^S(\widetilde{q})\right)\mathbf{1}_{\mathcal{K}_f^S}\otimes\mathbf{1}_{\mathbb{C}^2}\\ &\quad -\frac{1}{2}\mathbf{1}_{\mathcal{K}_f^S}\otimes\left(B(p)\cdot\boldsymbol{\sigma}\right),\end{aligned}$$

where $\widetilde{q} = q - A(p)$, $\nu,\mu = 1,2$. F_{Lor}^S, $\mathcal{A}^S$ and $\mathcal{M}^S$ are defined by

$$F_{Lor}^S(k,p) := -\nabla\phi(p) + \nabla E_*^S(k)\times B(p),$$

$$\mathcal{A}^S(k) := i\left\langle \psi^S(k), \nabla_k\psi^S(k)\right\rangle_{\mathcal{H}_f}$$

and

$$\mathcal{M}^S(k) := \frac{i}{2}\left\langle \nabla_k\psi^S(k), \times(H_{per}^S(k) - E_*^S(k))\nabla_k\psi^S(k)\right\rangle_{\mathcal{H}_f}.$$

Proof. One has

$$\begin{aligned}\mathbf{h}_0\oplus\mathbf{0}_{\mathcal{K}_f^\perp} &= u_0H_0\pi_0u_0^*\\ &= u_0^SH_0^S\pi_0^Su_0^{S*}\otimes\mathbf{1}_{\mathbb{C}^2}\\ &= \left(\mathbf{h}_0^S\oplus\mathbf{0}_{\mathcal{K}_f^{S,\perp}}\right)\otimes\mathbf{1}_{\mathbb{C}^2}\\ &= \left(\mathbf{h}_0^S\otimes\mathbf{1}_{\mathbb{C}^2}\right)\oplus\mathbf{0}_{\mathcal{K}_f^{P,\perp}}\end{aligned}$$

where we identified

$$(\mathcal{K}_f^S\oplus\mathcal{K}_f^{S,\perp})\otimes\mathbb{C}^2 \cong (\mathcal{K}_f^S\otimes\mathbb{C}^2)\oplus\left(\mathcal{K}_f^{S,\perp}\otimes\mathbb{C}^2\right).$$

Furthermore

$$\begin{aligned}\mathbf{h}_1(q,p)\oplus\mathbf{0}_{\mathcal{K}_f^\perp} &= \left(u\sharp H_0\sharp\pi\sharp u^*\right)_1(q,p) + u_0H_1\pi_0u_0^*(q,p)\\ &= \left(u^S\sharp H_0^S\sharp\pi^S\sharp u^{S*}\right)_1(q,p)\otimes\mathbf{1}_{\mathbb{C}^2}\\ &\quad -\frac{1}{2}\left(u_0^S\otimes\mathbf{1}_{\mathbb{C}^2}\right)\left(\mathbf{1}_{\mathcal{H}_f^S}\otimes(B(p)\cdot\boldsymbol{\sigma})\right)\left(\pi_0^Su_0^{S*}\otimes\mathbf{1}_{\mathbb{C}^2}\right)\\ &= \left(\mathbf{h}_1^S\otimes\mathbf{1}_{\mathbb{C}^2}\right)\oplus\mathbf{0}_{\mathcal{K}_f^\perp} - \frac{1}{2}\left(\mathbf{1}_{\mathcal{K}_f^S}\otimes(B(p)\cdot\boldsymbol{\sigma})\right)\oplus\mathbf{0}_{\mathcal{K}_f^\perp}.\end{aligned}$$

The computation of $\mathbf{h}_0^S$ and $\mathbf{h}_1^S$ is as in chapter 2. ∎

Remark 3.7 *The Hamiltonian* $\mathbf{h}_0^S + \varepsilon \mathbf{h}_1^S$ *is just the effective Hamiltonian derived in [Teu], chapter* 5.

3.4 Semiclassical limit

As in chapter 2 one obtains, in the case of a single 2-fold degenerate eigenvalue band E_*, semiclassical equations of motion in the reference representation. The degeneracy is, as explained in lemma 3.5, of a particular simple form, i.e. it does not interact with the transformation between Zak and reference representation. Therefore, we can translate all our results back even to the physical representation, in contrast to chapter 2 where this was only possible in principal order for scalar-valued symbols. As to be explained in detail below, one arrives at the equations of motion

$$\begin{aligned} \dot{q} &= \nabla_\pi\big(E_*(\pi) - \varepsilon B(q)\cdot \mathcal{M}^S(\pi)\big) + \varepsilon \Omega_{\mathcal{A}^S}(\pi) \times \dot{\pi} \\ \dot{\pi} &= -\nabla_q\big(\phi(q) - \varepsilon B(q)\cdot \big(\mathcal{M}^S(\pi) + n\big)\big) + \varepsilon \dot{q} \times B(q) \\ \dot{n} &= n \times B(q). \end{aligned} \tag{3.6}$$

with $\Omega_{\mathcal{A}^S} := \nabla \times \mathcal{A}^S$ and $\mathcal{A}^S$, $\mathcal{M}^S$ as defined in corollary 3.6. To be precise, let $\tilde{\Phi}^{t,\varepsilon} = \left(\tilde{\Phi}^{t,\varepsilon}_q, \tilde{\Phi}^{t,\varepsilon}_\pi, \tilde{\Phi}^{t,\varepsilon}_n\right)$ be the flow generated on $\mathbb{R}^6 \times S^2$ by 3.6 and let

$$\Phi^{t,\varepsilon}(q,p,n) := \tilde{\Phi}^{t,\varepsilon}(q, p - A(q), n) + (0, A \circ \tilde{\Phi}^{t,\varepsilon}_q(q, q - A(p)), 0). \tag{3.7}$$

Then we have the following result for observables $\widehat{\mathbf{b}}$ that are the Weyl-quantizations of symbols $\mathbf{b} \in S^1(\mathbb{R}^6, \mathcal{L}(\mathbb{C}^2))$ and Γ^*-periodic in the second argument.

Theorem 3.8 *Let* E_* *be an isolated two-fold degenerate Bloch band and* $\Phi^{t,\varepsilon} = \left(\Phi^{t,\varepsilon}_{q,p}, \Phi^{t,\varepsilon}_n\right)$ *be defined as in (3.7). Let furthermore* $b \in C_b^\infty(\mathbb{R}^6 \times S^2, \mathbb{C})$ *be* Γ^**-periodic in the second argument, i.e.* $b(q, p+\gamma^*, n) = b(q,p,n)$*, let*

$$\Pi^\varepsilon := \left(\mathcal{U}^{-1} \otimes \mathbf{1}_{\mathbb{C}^2}\right) \Pi^\varepsilon_Z \left(\mathcal{U} \otimes \mathbf{1}_{\mathbb{C}^2}\right)$$

and

$$\mathbf{b}_\varepsilon(t) := 2 \int_{S^2} d\lambda(n) b \circ \Phi^{t,\varepsilon}(\cdot,\cdot,n) \left(\frac{1}{2}\mathbf{1}_{\mathbb{C}^2} + \sqrt{\frac{3}{4}} n \cdot \boldsymbol{\sigma}\right).$$

Then we have

$$\Pi^\varepsilon \left(\exp(iH^\varepsilon t/\varepsilon) \widehat{\mathbf{b}} \exp(-iH^\varepsilon t/\varepsilon) - \widehat{\mathbf{b}_0(t)}\right) \Pi^\varepsilon = \mathcal{O}(\varepsilon)$$

and, if b is independent of n,

$$\Pi^\varepsilon\left(\exp(iH^\varepsilon t/\varepsilon)\widehat{\mathbf{b}}\exp(-iH^\varepsilon t/\varepsilon)-\widehat{\mathbf{b}_\varepsilon(t)}\right)\Pi^\varepsilon=\mathcal{O}(\varepsilon^2)$$

uniformly for any finite time interval, with $\mathbf{b} := \mathbf{b}(0)$ *and the Weyl quantization in the sense of* $\widehat{\mathbf{b}} = \mathbf{b}(-i\nabla_x, \varepsilon x)$.

To prove the theorem, we use the same strategy as in chapter 2. First we do the semiclassical limit in the reference space, then we translate it back to Zak and physical representation. Since many of the steps are similar, we shortened the presentation except for the parts where substantial differences arise.

We start with introducing the same correspondence between $\mathcal{L}(\mathcal{K}_f^P) \cong \mathcal{L}(\mathcal{K}_f^S \otimes \mathbb{C}^2) \cong \mathcal{L}(\mathbb{C}^2)$-valued symbols on $\mathbb{R}^6$ and scalar-valued symbols on the larger phase space $\mathbb{R}^6 \times S^2$ as we did in section 2.3. Note that now the quantity $\mathbf{\Delta}(n)$ has the particular simple form

$$\mathbf{\Delta}(n) = \mathbf{1}_{\mathcal{K}_f^S} \otimes (\frac{1}{2}\mathbf{1}_{\mathbb{C}^2} + \sqrt{\frac{3}{4}}n\cdot\boldsymbol{\sigma}).$$

The effective Hamiltonian including the first order reads

$$h^\varepsilon(q,p,n) = h_0(q,p,n) + \varepsilon h_1(q,p,n)$$

with

$$\begin{aligned} h_0(q,p,n) &= \big(E_*^S(\widetilde{q}) + \phi(p)\big)\\ h_1(q,p,n) &= -F_{\mathrm{Lor}}^P(\widetilde{q},p)\cdot\mathcal{A}^S(\widetilde{q}) - B(p)\cdot\mathcal{M}^S(\widetilde{q}) + \frac{\sqrt{3}}{2}B(p)\cdot n. \end{aligned}$$

In analogy to the results in section 2.3 we first get the equations of motion in the reference space as

$$\begin{aligned} \dot{q} &= -\nabla_p h^\varepsilon(q,p,n)\\ \dot{p} &= \nabla_q h^\varepsilon(q,p,n)\\ \dot{n} &= n\times B(p). \end{aligned}$$

resp. the equations of motion in terms of the kinetic momentum as

$$\begin{aligned} \dot{\widetilde{q}} &= -\nabla\phi(p) + \dot{p}\times B(p) + \varepsilon\frac{\sqrt{3}}{2}\nabla_p\left(B(p)\cdot n\right)\\ &\quad +\varepsilon\nabla_p\left(F_{\mathrm{Lor}}(\widetilde{q},p)\cdot\mathcal{A}^S(\widetilde{q}) + B(p)\cdot\mathcal{M}^S(\widetilde{q})\right)\\ \dot{p} &= \nabla E(\widetilde{q}) - \varepsilon\nabla_{\widetilde{q}}\left(F_{\mathrm{Lor}}(\widetilde{q},p)\cdot\mathcal{A}^S(\widetilde{q}) + B(p)\cdot\mathcal{M}^S(\widetilde{q})\right)\\ \dot{n} &= n\times B(p). \end{aligned}$$

The translation of the equations back to the Zak representation requires some care, therefore, we give a proof of the following lemma which is in principle analogue to lemma 2.20

Lemma 3.9 *Let* $\mathbf{a} \in S^{\mathbf{1}}(\varepsilon, \mathcal{L}(\mathcal{K}_f))$ *with* a_0 *independent of* n *and*

$$\mathbf{b} := u^* \sharp \left(\mathbf{a} \oplus \mathbf{0}\right) \sharp u.$$

Then

$$\mathbf{a} = 2 \int_{S^2} d\lambda(n) \left(b \circ T_+\right)(\cdot, \cdot, n) \boldsymbol{\Delta}(n) + \mathcal{O}(\varepsilon^2)$$

and vice versa

$$\mathbf{b} = 2 \int_{S^2} d\lambda(n) \left(a \circ T_-\right)(\cdot, \cdot, n) \widetilde{\boldsymbol{\Delta}}(n) + \mathcal{O}(\varepsilon^2)$$

with

$$T_\pm(q,p,n) = (q \pm \varepsilon \left(\nabla A\right)^\top \mathcal{A}(q - A(p)), p \pm \varepsilon \mathcal{A}(q - A(p)), n),$$

$$\widetilde{\boldsymbol{\Delta}}(n) = \pi^S \otimes (\frac{1}{2}\mathbf{1}_{\mathbb{C}^2} + \sqrt{\frac{3}{4}} n \cdot \boldsymbol{\sigma})$$

and

$$b(q,p,n) := Tr(\mathbf{b}(q,p)\tilde{\boldsymbol{\Delta}}(q,p,n)).$$

Proof. We have

$$\begin{aligned}
\mathbf{b} &= u^* \sharp \left(\mathbf{a} \oplus \mathbf{0}\right) \sharp u \\
&= 2 \int_{S^2} \mathrm{d}\lambda(n) u^* \sharp a(\cdot, \cdot, n) \sharp u \sharp u^* \sharp \left(\boldsymbol{\Delta}(n) \oplus \mathbf{0}\right) \sharp u \\
&=: 2 \int_{S^2} \mathrm{d}\lambda(n) u^* \sharp a(\cdot, \cdot, n) \sharp u \sharp \widetilde{\boldsymbol{\Delta}}(n) \\
&= 2 \int_{S^2} \mathrm{d}\lambda(n) \left(\left(u^{S*} \sharp a(\cdot, \cdot, n) \sharp u^S\right) \otimes \mathbf{1}_{\mathbb{C}^2}\right) \sharp \widetilde{\boldsymbol{\Delta}}(n)
\end{aligned}$$

where we used lemma 3.5. Now, as in lemma 2.20 one shows that

$$u^{S*} \sharp a(\cdot, \cdot, n) \sharp u^S = a \circ T_-(\cdot, \cdot, n) + \mathcal{O}(\varepsilon^2).$$

Furthermore, one has

$$
\begin{aligned}
& u^* \sharp \left(\mathbf{\Delta}(n) \oplus \mathbf{0}\right) \sharp u \\
&= \left(u^{S*} \otimes \mathbf{1}_{\mathbb{C}^2}\right) \sharp \left(\left(\mathbf{1}_{\mathcal{K}_f^S} \oplus \mathbf{0}_{\mathcal{K}_f^{S,\perp}} \right) \otimes \left(\frac{1}{2}\mathbf{1}_{\mathbb{C}^2} + \sqrt{\frac{3}{4}} n \cdot \boldsymbol{\sigma}\right) \right) \sharp \left(u^S \otimes \mathbf{1}_{\mathbb{C}^2}\right) \\
&= \left(u^{S*} \sharp \left(\mathbf{1}_{\mathcal{K}_f^S} \oplus \mathbf{0}_{\mathcal{K}_f^{S,\perp}} \right) \sharp u^S \right) \otimes \left(\frac{1}{2}\mathbf{1}_{\mathbb{C}^2} + \sqrt{\frac{3}{4}} n \cdot \boldsymbol{\sigma}\right) \\
&= \pi^S \otimes \left(\frac{1}{2}\mathbf{1}_{\mathbb{C}^2} + \sqrt{\frac{3}{4}} n \cdot \boldsymbol{\sigma}\right).
\end{aligned}
$$

Moyal-multiplying from both sides with u^* and u gives the second statement. ■

Now, as in section 2.3 one can translate the equations back to the Zak representation and has the equations

$$
\begin{aligned}
\dot{\tilde{q}} &= -\nabla_p(\phi(p) - \varepsilon B(p) \cdot \left(\mathcal{M}^S(\tilde{q}) + n\right)) + \varepsilon \dot{p} \times B(p) \\
\dot{p} &= \nabla_{\tilde{q}}(E(\tilde{q}) - \varepsilon B(p) \cdot \mathcal{M}^S(\tilde{q})) + \varepsilon \Omega_{\mathcal{A}^S}(\tilde{q}) \times \dot{\tilde{q}} \\
\dot{n} &= n \times B(p).
\end{aligned}
\tag{3.8}
$$

Not surprising, the first two equations in (3.8) are the equations of motion derived in [Teu], chapter 5, except for the fact that we have an additional term coming from the subprincipal symbol H_1 of the original Hamiltonian. If we call the corresponding flow as $\tilde{\Phi}_Z^{t,\varepsilon}$ resp. the flow in physical coordinates as $\Phi_Z^{t,\varepsilon}$, i.e.

$$
\Phi_Z^{t,\varepsilon}(q,p,n) = \tilde{\Phi}_Z^{t,\varepsilon}(q - A(p), p, n) + (A \circ \tilde{\Phi}_{Z,p}^{t,\varepsilon}(q - A(p)), 0, 0), \tag{3.9}
$$

then we have (as in chapter 2) the following result.

Proposition 3.10 *Let $|\mathcal{I}| = 2$, i.e. E_* is an isolated two-fold degenerate Bloch band and $\Phi_Z^{t,\varepsilon}$ be defined as in (3.9). Let furthermore $b \in C_b^\infty(\mathbb{R}^6 \times S^2, \mathbb{C})$ and $\mathbf{b} \in S^{\mathbf{1}}(\mathbb{R}^6, \mathcal{L}(\mathcal{H}_f^P))$ be given by*

$$
\mathbf{b}_\varepsilon(t) := 2 \int_{S^2} d\lambda(n) \left(b \circ \Phi_Z^{t,\varepsilon}\right) \mathbf{1}_{\mathcal{H}_f^S} \otimes \left(\frac{1}{2}\mathbf{1}_{\mathbb{C}^2} + \sqrt{\frac{3}{4}} n \cdot \boldsymbol{\sigma}\right)
$$

Then we have

$$
\Pi_Z^\varepsilon \left(\exp(iH_Z^\varepsilon t/\varepsilon) \widehat{\mathbf{b}} \exp(-iH_Z^\varepsilon t/\varepsilon) - \widehat{\mathbf{b}_0(t)} \right) \Pi_Z^\varepsilon = \mathcal{O}(\varepsilon)
$$

and, if b is independent of n,

$$
\Pi_Z^\varepsilon \left(\exp(iH_Z^\varepsilon t/\varepsilon) \widehat{\mathbf{b}} \exp(-iH_Z^\varepsilon t/\varepsilon) - \widehat{\mathbf{b}_\varepsilon(t)} \right) \Pi_Z^\varepsilon = \mathcal{O}(\varepsilon^2)
$$

with $\widehat{\mathbf{b}} := \widehat{\mathbf{b}}(0)$uniformly for any finite time interval.

Proof. The derivation of the semiclassical limit in the reference space is exactly as in chapter 2. For translating the result back to the Zak representation, we observe that lemma 2.20 is valid as well because of lemma 3.5. ■

Now we can give the proof of theorem 3.8.

Proof. (of theorem 3.8) We insert $\mathcal{U}^{-1}\otimes\mathbf{1}_{\mathbb{C}^2}$ and $\mathcal{U}\otimes\mathbf{1}_{\mathbb{C}^2}$ between the quantities of proposition 3.4. By definition we have

$$\Pi^\varepsilon = \left(\mathcal{U}^{-1}\otimes\mathbf{1}_{\mathbb{C}^2}\right)\Pi^\varepsilon_Z\left(\mathcal{U}\otimes\mathbf{1}_{\mathbb{C}^2}\right)$$

and

$$\exp(iH^\varepsilon t/\varepsilon) = \left(\mathcal{U}^{-1}\otimes\mathbf{1}_{\mathbb{C}^2}\right)\exp(iH^\varepsilon_Z t/\varepsilon)\left(\mathcal{U}\otimes\mathbf{1}_{\mathbb{C}^2}\right).$$

Furthermore we have

$$\begin{aligned}&\left(\mathcal{U}^{-1}\otimes\mathbf{1}_{\mathbb{C}^2}\right)\mathcal{W}\left(2\int_{S^2}\mathrm{d}\lambda(n)b\circ\Phi^{t,\varepsilon}(\cdot,\cdot,n)\boldsymbol{\Delta}(q,p,n)\right)\left(\mathcal{U}\otimes\mathbf{1}_{\mathbb{C}^2}\right)\\ &= 2\int_{S^2}\mathrm{d}\lambda(n)\left(\mathcal{U}^{-1}\mathcal{W}\left(b\circ\Phi^{t,\varepsilon}(\cdot,\cdot,n)\mathbf{1}_{\mathcal{H}^S_f}\right)\mathcal{U}\right)\otimes\left(\frac{1}{2}\mathbf{1}_{\mathbb{C}^2}+\sqrt{\frac{3}{4}}n\cdot\boldsymbol{\sigma}\right)\end{aligned}$$

including the cases $\varepsilon = 0$ and $t = 0$ (the latter one leading to $\widehat{\mathbf{b}}$). Now as in chapter 2 the result follows with proposition 5.21 in [Teu]. ■

3.5 Adiabatic perturbation theory with relativistic corrections

In section 3.1 we stated a theorem relating the time evolution of the Dirac Hamiltonian with the one of the Pauli Hamiltonian. Unfortunately, we were not able to prove such a relation including relativistic corrections of higher orders. However, one can, as done in the physics literature derive relativistic corrections to the Pauli Hamiltonian at least on a formal level. The resulting Hamiltonian derived in [Yn], p. 84 reads in our case

$$\begin{aligned}H^{\varepsilon,sr} \;:&= H^{\varepsilon,P} - \frac{1}{8c^2}((-i\nabla_x - A(\varepsilon x))^2 - \varepsilon B(\varepsilon x)\cdot\boldsymbol{\sigma})^2\\ &+\frac{1}{8c^2}\left((\nabla V_\Gamma(x)+\varepsilon\nabla\phi(\varepsilon x))\times(-i\nabla_x)\cdot\boldsymbol{\sigma} - \Delta V_\Gamma(x) - \varepsilon^2\Delta\phi(\varepsilon x)\right).\end{aligned}$$

The unperturbed Hamiltonian in Bloch-Flouquet representation reads in this case

$$\begin{aligned}H^{sr}_{\mathrm{per}}(k) &= \frac{1}{2}(-i\nabla_y+k)^2 + V_\Gamma(y) - \frac{1}{8c^2}(-i\nabla_y+k)^4\\ &+\frac{1}{8c^2}\nabla V_\Gamma(y)\times(-i\nabla_y+k)\cdot\boldsymbol{\sigma} - \frac{1}{8c^2}\Delta V_\Gamma(x).\end{aligned}$$

Under suitable additional assumptions on V_Γ, $H^{sr}_{per}(k)$ is self-adjoint with domain $\mathcal{D} := H^4(\mathbb{T}^3) \otimes \mathbb{C}^2 \subset L^2(\mathbb{T}^3) \otimes \mathbb{C}^2$ and one can apply space-adiabatic perturbation theory as in the Dirac or Pauli case. The resulting effective Hamiltonian yields

$$(\mathbf{h}^{sr}_0)_{\nu,\mu}(q,p) = \left\langle \psi^{sr}_\nu(q - A(p)), H^{sr}_0(q,p)\psi^{sr}_\mu(q - A(p)) \right\rangle, \quad \nu,\mu \in \{1,\dots,N\}$$

with

$$H^{sr}_0(q,p) = H^P_0 - \frac{1}{8c^2}(-i\nabla_y + q - A(p))^4 + \frac{1}{8c^2}\left(\nabla V_\Gamma(y) \times (-i\nabla_y) \cdot \boldsymbol{\sigma} - \Delta V_\Gamma(y)\right)$$

and $\psi^{sr}_\nu(k)$ eigenfunctions of the unperturbed Hamiltonian $H^{sr}_{\mathrm{per}}(k)$. As in the Dirac and Pauli case, one can compute the first order corrections in the case of a single two-fold degenerate eigenvalue band $E_*(k)$ as

$$\begin{aligned}(\mathbf{h}_1)_{\nu,\mu}(q,p) &= -F_{\mathrm{Lor}}(\widetilde{q},p) \cdot \mathcal{A}^{sr}_{\nu,\mu}(\widetilde{q}) - B(p) \cdot \mathcal{M}^{sr}_{\nu,\mu}(\widetilde{q}) \\ &\quad + \left\langle \psi^{sr}_\nu(q - A(p)), H^{sr}_1(q,p)\psi^{sr}_\mu(q - A(p)) \right\rangle.\end{aligned}$$

where $\widetilde{q} = q - A(p)$, $\nu,\mu = 1,\dots,N$. F_{Lor}, $\mathcal{A}$ and $\mathcal{M}$ are defined analogously to the Dirac resp. Pauli case and H^{sr}_1 is given by

$$\begin{aligned}H^{sr}_1(q,p) &= -\frac{1}{2}B(p) \cdot \boldsymbol{\sigma} - \frac{1}{4c^2}(-i\nabla_y + q - A(p))^2(B(p) \cdot \boldsymbol{\sigma}) \\ &\quad + \frac{1}{8c^2}\nabla\phi(p) \times (-i\nabla_y + q) \cdot \boldsymbol{\sigma}.\end{aligned}$$

Due to the spin-orbit term $\nabla V_\Gamma(y) \times (-i\nabla_y + k) \cdot \boldsymbol{\sigma}$, that appears already in the unperturbed Hamiltonian, one has no special symmetry in the eigenfunctions of a band as one had in the Pauli case for $|\mathcal{I}| = 2$. Therefore, the results do not provide new insight compared to the Dirac case.

4 Nonrelativistic limit of Dirac-Bloch electrons

After having studied the adiabatic limit of the Pauli Hamiltonian, it is natural to ask whether all the quantities in chapter 2 have a limit as c tends to ∞ and whether this limit agrees with the corresponding quantities derived from the Pauli Hamiltonian. To fix notation, we put a super- or subscript P on the quantities of chapter 3 and make the c-dependence of the quantities of chapter 2 explicit either by putting a superscript c or writing the quantity as a function of c. The keystone for our analysis is, as in section 3.1, the fact that the c-dependent resolvent $R_{\mathrm{per}}(\zeta, k, c)$ as introduced in (2.6) has for fixed (ζ, k) a power series expansion around $c = \infty$ of the form

$$R_{\mathrm{per}}(\zeta + c^2, k, c) = \sum_{n=0}^{\infty} \frac{1}{c^n} R_{\mathrm{per},n}(\zeta, k)$$

for c large enough according to [Th]. An analysis of the proof of Thaller in section 4.1 shows that in our case the power series converges not only pointwise, but can be also differentiated coefficientwise with respect to k and ζ and that the power series of the derivatives converge uniformly in $k \in M^*$, $\zeta \in \Lambda_{\mathrm{per}}(k)$ for $\frac{1}{c}$ small enough. Moreover, one can even give a lower bound R on the radius of convergence independent of the degree of the derivatives. In particular, for $\frac{1}{c} \leq R$, the existence of an isolated family $\{E_n(k, c)\}_{n \in \mathcal{I}}$ enclosed by circles $\Lambda^P_{\mathrm{per}}(k) + c^2$ with Λ^P_{per} from chapter 3 independent of c follows. Furthermore also $P_{\mathrm{per}}(k, c)$, the unitary $U_{\mathrm{per}}(k, c)$ and their derivatives have uniformly convergent power series expansions for $\frac{1}{c} \leq R$.

Next, in section 4.2 we will study how these results are related to the symbols $\pi(c), u(c)$ and $h(c)$ resp. their quantizations. To make the quantities comparable, one chooses as reference space the reference space of the Pauli Hamiltonian. Then one can show that $\pi(c)$, $u(c)$ and $h(c) - c^2$ have, for $\frac{1}{c} \leq R$ power series expansions in $\frac{1}{c}$ that are absolutely convergent in $\|\cdot\|_n^{(\mathbf{1})}$ for any $n \in \mathbb{N}$, which translates to a norm-convergent power series expansion for their quantizations. The result is given in theorem 4.4. An obvious question is also whether the central statements of theorem 2.6, i.e.

$$\|[\exp(-iH_Z^\varepsilon t), \Pi_Z^\varepsilon]\| = \mathcal{O}(\varepsilon^\infty(1+|t|))$$

and

$$\left\|\exp(-iH_Z^\varepsilon t)\Pi_Z^\varepsilon - U^{\varepsilon *}\left(\exp(-i\widehat{\mathbf{h}}t) \oplus \mathbf{0}\right) U^\varepsilon\right\| = \mathcal{O}(\varepsilon^\infty(1+|t|))$$

hold uniformly in c. Unfortunately they don't need to, but one can at least show that the error term is at most linearly growing in c as stated in theorem 4.4.

Finally we also study the behavior of the semiclassical limit. In particular, theorem 4.7 tells us that one can approximate the time evolution of an observable under the Dirac Hamiltonian by the semiclassical equations of motion derived from the Pauli Hamiltonian.

4.1 The unperturbed quantities

As mentioned in the introduction of this chapter, we first concentrate on an expansion of the unperturbed resolvent $R_{\mathrm{per}}(\zeta + c^2, k, c)$ and the existence of an isolated family $\{E_n(c)\}_{n\in\mathcal{I}}$ in a neighborhood of $c = \infty$. After that we focus on the projection $P_{\mathrm{per}}(k,c)$ and in particular on the τ-equivariant unitary $U_{\mathrm{per}}(k,c)$.

As a start, we fix an isolated family $\{E_n^P(k)\}_{n\in\mathcal{I}}$ of eigenvalue bands of the Pauli Hamiltonian and enclosing circles $\Lambda_{\mathrm{per}}^P(k)$ as in chapter 3. In the following, we will deal with the Hamiltonian

$$H_{\mathrm{per}}^\infty(k) := H_{\mathrm{per}}^P(k) \otimes \frac{1}{2}(-i\nabla_y - k)^2$$

self-adjoint on $\mathcal{D}^P \otimes \mathcal{D}^P =: \mathcal{D}^\infty \subset \mathcal{H}_f^\infty = \mathcal{H}_f^P \otimes \mathcal{H}_f^P$ and its resolvent

$$R_{\mathrm{per}}^\infty(\zeta, k) := \left(H_{\mathrm{per}}^\infty(k) - \zeta\right)^{-1}.$$

Therefore it will turn out useful to assume that

$$\inf_{k\in M^*} dist(\Lambda_{\mathrm{per}}^P(k), \sigma(H_{\mathrm{per}}^\infty(k))) > 0.$$

Note that this condition on Λ_{per}^P is stricter than the one introduced in chapter 3, but since $\frac{1}{2}(-i\nabla_y + k)^2$ has for fixed $k \in M^*$ purely discrete spectrum accumulating at infinity and it was not required for Λ_{per}^P to be continuous, this can be satisfied without further problems. Furthermore we choose $O_{\mathrm{per}}^P \subset \mathbb{C}\times\mathbb{R}^3$ and $K_{\mathrm{per}}^P \subset \mathbb{C}\times\mathbb{R}^3$ such that

$$\bigcup_{k\in\mathbb{R}^3}\left(\Lambda_{\mathrm{per}}^P(k) \times \{k\}\right) \subset K_{\mathrm{per}}^P \subset O_{\mathrm{per}}^P \subset \bigcup_{k\in\mathbb{R}^3}\left(\mathbb{C}\setminus\sigma(H_{\mathrm{per}}^\infty(k)) \times \{k\}\right).$$

Finally, we introduce the projectors

$$\begin{aligned}\pi_+ &= \mathbf{1}_{L^2(\mathbb{T}^3)} \otimes (\mathbf{1}_{\mathbb{C}^2} \oplus \mathbf{0}_{\mathbb{C}^2}),\\ \pi_- &= \mathbf{1} - \pi_+\end{aligned}$$

on the upper resp. lower components. The quantizations of $\pi_\pm$ (precisely: of the symbols $(q,p) \mapsto \pi_\pm$) are $P_\pm := \widehat{\pi}_\pm$. In the following, we will frequently use the splitting of an operator $A \in \mathcal{L}(\mathcal{H}_f)$ into its diagonal resp. even part

$$A^D = \pi_+ A \pi_+ + \pi_- A \pi_-$$

and its off-diagonal resp. odd part

$$A^{OD} = \pi_+ A \pi_- + \pi_- A \pi_+.$$

Now we turn to the expansion of $R_{\mathrm{per}}(\zeta + c^2, k, c)$ starting with the following lemma.

Lemma 4.1 *Let* $K(\zeta,k,c) := \left(\mathbf{1} - \frac{1}{2c^2}\zeta^2 R^\infty_{per}(\zeta,k)\right)^{-1} R^\infty_{per}(\zeta,k)$. *Then* $K(\zeta,k,c)$ *is well defined for* $c > \sqrt{\frac{1}{2}|\zeta|^2 \left\| R^\infty_{per}(\zeta,k)\right\|_{\mathcal{L}(\mathcal{H}_f^\infty,\mathcal{D}^\infty)}}$ *and has the power series expansion*

$$K(\zeta,k,c) = \sum_{n=0}^\infty \frac{1}{c^{2n}} \frac{\zeta^2}{2} \left(\frac{\zeta^2}{2} R^\infty_{per}(\zeta,k)\right)^{n+1}.$$

Moreover, for any $\alpha \in \mathbb{N}_0 \times \mathbb{N}_0^3$ *the series converges absolutely in the sense of* $\sup_{(\zeta,k)\in K^P_{per}} \left\| \partial^\alpha_{(\zeta,k)} \cdot \right\|_{\mathcal{L}(\mathcal{H}_f^\infty,\mathcal{D}^\infty)}$ *for*

$$c > \sqrt{\sup_{(\zeta,k)\in K^P_{per}} \left\| \frac{1}{2}|\zeta|^2 R^\infty_{per}(\zeta,k)\right\|_{\mathcal{L}(\mathcal{H}_f^\infty,\mathcal{D}^\infty)}}$$

Proof. Clearly, for fixed $(\zeta,k) \in O^P_{\mathrm{per}}$ and $c > \sqrt{\frac{1}{2}|\zeta|^2 \left\| R^\infty_{\mathrm{per}}(\zeta,k)\right\|_{\mathcal{L}(\mathcal{H}_f^\infty,\mathcal{D}^\infty)}}$, we can expand $\left(\mathbf{1} - \frac{1}{2c^2}\zeta^2 R^\infty_{\mathrm{per}}(\zeta,k)\right)^{-1}$ into a von Neumann series that converges in $\|\cdot\|_{\mathcal{L}(\mathcal{H}_f^\infty)}$. It remains to show that the series converges in the sense of

$$\sup_{(\zeta,k)\in K^P_{\mathrm{per}}} \left\| \partial^\alpha_{(\zeta,k)} \cdot \right\|_{\mathcal{L}(\mathcal{H}_f^\infty,\mathcal{D}^\infty)}.$$

To this end, we fix $l \in \mathbb{N}$ and observe

$$\begin{aligned}&\partial^\alpha_{(\zeta,k)} \left(\frac{\zeta^2}{2} R^\infty_{\mathrm{per}}(\zeta,k)\right)^l\\ &= \sum_{\alpha^{(1)}+\dots+\alpha^{(l)}=\alpha} \frac{\alpha!}{\alpha^{(1)}!\dots\alpha^{(l)}!} \prod_{i=1}^l \partial^{\alpha^{(i)}}_{(\zeta,k)} \left(\frac{\zeta^2}{2} R^\infty_{\mathrm{per}}(\zeta,k)\right).\end{aligned}$$

For $l > |\alpha|$ every summand has at most $|\alpha|$ factors that with $\alpha^{(i)} \neq 0$, therefore we have the norm estimate

$$\left\| \partial^\alpha_{(\zeta,k)} \left(\frac{\zeta^2}{2} R^\infty_{\text{per}}(\zeta,k) \right)^l \right\| \leq l^{|\alpha|} C_\alpha \left\| \frac{\zeta^2}{2} R^\infty_{\text{per}}(\zeta,k) \right\|^{l-|\alpha|}_{\mathcal{L}(\mathcal{H}^\infty_f,\mathcal{D}^\infty)}$$

with

$$C_\alpha := \left(1 + \sup_{(\zeta,k)\in K^P_{\text{per}}} \sup_{\beta\leq\alpha} \left\| \partial^\beta_{(\zeta,k)} \frac{\zeta^2}{2} R^\infty_{\text{per}}(\zeta,k) \right\|_{\mathcal{L}(\mathcal{H}^\infty_f,\mathcal{D}^\infty)} \right)^{|\alpha|} < \infty.$$

$C_\alpha < \infty$ can be seen inductively by noticing that K^P_{per} is compact, $R^\infty_{\text{per}}(\zeta,k) \in \mathcal{L}(\mathcal{H}^\infty_f, \mathcal{D}^\infty)$ and differentiating the relation $(H^\infty_{\text{per}}(k)-\zeta)R^\infty_{\text{per}}(\zeta,k) = \mathbf{1}$ from which one obtains

$$\partial^\alpha_{(\zeta,k)} R^\infty_{\text{per}}(\zeta,k) = -R^\infty_{\text{per}}(\zeta,k) \sum_{\beta\leq\alpha,\beta\neq 0} \binom{\alpha}{\beta} \partial^\beta_{(\zeta,k)} \left(H^\infty_{\text{per}}(k) - \zeta \right) \partial^{\alpha-\beta}_{(\zeta,k)} R^\infty_{\text{per}}(\zeta,k).$$

Now the claim follows by observing that the radius of convergence of the power series $\sum_{l=0}^\infty l^{|\alpha|} x^l$ is 1 independent of α. ■

Proposition 4.2 *For each fixed $(\zeta,k) \in O^\infty_{per}$ and all $\alpha \in \mathbb{N}^3_0 \times \mathbb{N}_0$, $\partial^\alpha_{(\zeta,k)} R_{per}(\zeta + c^2, k, c)$ is well-defined for $\frac{1}{c}$ small enough and has a power series expansion*

$$\partial^\alpha_{(\zeta,k)} R_{per}(\zeta + c^2, k, c) = \sum_{n=0}^\infty \frac{1}{c^n} \partial^\alpha_{(\zeta,k)} R_{per,n}(\zeta,k).$$

Moreover, the series converges absolutely in the sense of $\sup_{(\zeta,k)\in K^P_{per}} \left\| \partial^\alpha_{(\zeta,k)} \cdot \right\|_{\mathcal{L}(\mathcal{H}_f,\mathcal{D})}$ *with convergence radius R independent of α. The first two coefficients are given by*

$$\begin{aligned} R_{per,0}(\zeta,k) &= R^P_{per}(\zeta,k) \otimes \mathbf{0}, \\ R_{per,1}(\zeta,k) &= \frac{1}{2} \begin{pmatrix} \mathbf{0} & R^P_{per}(\zeta,k)\left((-i\nabla_y + k)\cdot\boldsymbol{\sigma}\right) \\ \left((-i\nabla_y + k)\cdot\boldsymbol{\sigma}\right) R^P_{per}(\zeta,k) & \mathbf{0} \end{pmatrix}. \end{aligned}$$

Proof. According to [Th], one has the identity

$$\begin{aligned} & R_{\text{per}}(\zeta + c^2, k, c) \\ &= \left(P_+ + \frac{1}{2c}\left(\alpha\cdot(-i\nabla_y - k) + \frac{1}{c}\zeta \right) \right) K(\zeta,k,c) \\ &\quad \times \left(\mathbf{1} + \frac{1}{2c} V_\Gamma(y) \left(\alpha\cdot(-i\nabla_y - k) + \frac{1}{c}\zeta \right) K(\zeta,k,c) \right)^{-1} \end{aligned} \tag{4.1}$$

whenever the right hand side is well-defined. For fixed (ζ, k) the last factor can be expanded into a von Neumann series

$$\begin{aligned}&\left(\mathbf{1} + \frac{1}{2c}V_\Gamma(y)\left(\alpha\cdot(-i\nabla_y - k) + \frac{1}{c}\zeta\right)K(\zeta,k,c)\right)^{-1} \\ &= \sum_{n=0}^{\infty}\frac{1}{c^n}\left(\frac{1}{2}V_\Gamma(y)\left(\alpha\cdot(-i\nabla_y - k) + \frac{1}{c}\zeta\right)K(\zeta,k,c)\right)^{l}\end{aligned} \tag{4.2}$$

whenever c is large enough that

$$\frac{1}{c}\left\|\frac{1}{2}V_\Gamma(y)\left(\alpha\cdot(-i\nabla_y - k) + \frac{1}{c}\zeta\right)K(\zeta,k,c)\right\|_{\mathcal{L}(\mathcal{H}_f)} < 1.$$

Note that such a c exists since $\|K(\zeta,k,c)\|_{\mathcal{L}(\mathcal{H}_f,\mathcal{D}^\infty)}$ stays bounded for large c (as it is a power series in $\frac{1}{c}$ for c large enough) and $V_\Gamma(y)(-i\nabla_y\cdot\alpha)$ as well as $V_\Gamma(y)$ are bounded operators in $\mathcal{L}(\mathcal{D}^\infty,\mathcal{H}_f)$ by assumption $(A1)$. Together with the series expansion of $K(\zeta,k,c)$ in lemma 4.1 it follows that $R_{\text{per}}(\zeta+c^2,k,c)$ has a (a priori pointwise) power series expansion

$$R_{\text{per}}(\zeta + c^2, k, c) = \sum_{n=0}^{\infty}\frac{1}{c^n}R_{\text{per},n}(\zeta,k). \tag{4.3}$$

The first two coefficients follow by direct computation as in [Th].

Next we show that (4.3) converges in $\sup_{(\zeta,k)\in K^P_{\text{per}}}\left\|\partial^\alpha_{(\zeta,k)}\cdot\right\|_{\mathcal{L}(\mathcal{H}_f,\mathcal{D})}$ with convergence radius R_α depending on α. To this end let, for $\frac{1}{c} < R_\alpha$, $K(\zeta,k,c)$ converge in $\sup_{(\zeta,k)\in K^P_{\text{per}}}\left\|\partial^\beta_{(\zeta,k)}\cdot\right\|_{\mathcal{L}(\mathcal{H}_f,\mathcal{D})}$ for all $\beta\leq\alpha$,

$$\sup_{(\zeta,k)\in K^P_{\text{per}}}\sup_{\beta\leq\alpha}\left\|\partial^\beta_{(\zeta,k)}K(\zeta,k,c)\right\|_{\mathcal{L}(\mathcal{H}_f,\mathcal{D}^\infty)} < 1$$

and

$$\frac{1}{c}\sup_{(\zeta,k)\in K^P_{\text{per}}}\sup_{\beta\leq\alpha}\left\|\partial^\beta_{(\zeta,k)}\frac{1}{2}V_\Gamma(y)\left(\alpha\cdot(-i\nabla_y - k) + \frac{1}{c}\zeta\right)\right\|_{\mathcal{L}(\mathcal{D}^\infty,\mathcal{H}_f)} < 1.$$

Then also (4.3) converges in $\sup_{(\zeta,k)\in K^P_{\text{per}}}\left\|\partial^\beta_{(\zeta,k)}\cdot\right\|_{\mathcal{L}(\mathcal{H}_f,\mathcal{D})}$ for all $\beta\leq\alpha$, in particular

$$\partial^\alpha_{(\zeta,k)}R_{\text{per}}(\zeta + c^2, k, c) = \sum_{n=0}^{\infty}\frac{1}{c^n}\partial^\alpha_{(\zeta,k)}R_{\text{per},n}(\zeta,k). \tag{4.4}$$

Finally, we show that there is even a α-independent lower bound R on the radius of convergence. One observes that the derivatives of $R_{\text{per}}(\zeta,k,c)$ satisfy

$$\begin{aligned}&\partial^{\alpha}_{(\zeta,k)}R_{\text{per}}(\zeta+c^2,k,c)\\ &= -R_{\text{per}}(\zeta+c^2,k,c)\sum_{\beta\le\alpha,\beta\neq 0}\binom{\alpha}{\beta}\partial^{\beta}_{(\zeta,k)}\left(H_{\text{per}}(k,c)-\zeta\right)\partial^{\alpha-\beta}_{(\zeta,k)}R_{\text{per}}(\zeta+c^2,k,c).\end{aligned}$$

Inductively it follows that $\partial^{\alpha}_{(\zeta,k)}R_{\text{per}}(\zeta+c^2,k,c)$ is a sum of compositions of the derivatives of $H_{\text{per}}(k,c)-\zeta$ (that are either $\mathbf{1}$ or $c\alpha_i$) and the resolvent $R_{\text{per}}(\zeta+c^2,k,c)$ itself. This sum of compositions expands therefore into a polynomial in c and a power series in $\frac{1}{c}$ that converges absolutely in $\sup_{(\zeta,k)\in K^P_{\text{per}}}\|\cdot\|_{\mathcal{L}(\mathcal{H}_f,\mathcal{D})}$ for $\frac{1}{c}\le R_0 =: R$. By uniqueness of the power series expansion this expansion and (4.4) must agree, therefore it follows that the power series (4.3) converges in $\sup_{(\zeta,k)\in K^P_{\text{per}}}\left\|\partial^{\alpha}_{(\zeta,k)}\cdot\right\|_{\mathcal{L}(\mathcal{H}_f,\mathcal{D})}$ for $\frac{1}{c}\le R$. ■

This proposition gives us also information about the existence of a c-dependent isolated family.

Corollary 4.3 *Let $\{E^P_n(k)\}_{n\in\mathcal{I}}$ be an isolated family of eigenvalue bands of the Pauli Hamiltonian. Then, for $\frac{1}{c}\le R$, the family $\{E_n(k,c)\}_{n\in\mathcal{I}}$ is also isolated and enclosed by the circle $\Lambda^P_{per}(k)+c^2$. In particular, all the quantities of chapter 2 can be constructed for $\frac{1}{c}\le R$.*

Proof. We recall that $\Lambda^P_{\text{per}}(k)+c^2$ can be chosen to be locally constant in k. Since $R_{\text{per}}(\cdot,k,c)$ is defined on $\Lambda^P_{\text{per}}(k)+c^2$ for $k\in M^*$, $\frac{1}{c}\le R$ by proposition 4.2, we know that

$$\begin{aligned}P_{\text{per}}(k,c) &= \int_{\Lambda_{\text{per}}(k)+c^2}\mathrm{d}\zeta R_{\text{per}}(\zeta,k,c)\\ &= \int_{\Lambda_{\text{per}}(k)}\mathrm{d}\zeta R_{\text{per}}(\zeta+c^2,k,c)\end{aligned}$$

is for all $k\in M^*, \frac{1}{c}\le R$ an projector of (by local continuity in k) constant dimension d and that $\Lambda^P_{\text{per}}(k)+c^2$ separates d bands of eigenvalues (resp. bands whose degree of degeneracy add up to d) from the rest of the spectrum. This family must necessarily be isolated. Furthermore, the indices of the families $\{E^P_n(k)\}_{n\in\mathcal{I}}$ and its corresponding $c$dependent family (i.e. the set $\mathcal{I}$) are the same since $E_1(k,c)$ was defined as the lowest eigenvalue greater than 0 as in the case of the Pauli Hamiltonian. ■

It remains to show that also $P_{\text{per}}(k,c)$ and $U_{\text{per}}(k,c)$ have power series expansions in $\frac{1}{c}$. For $P_{\text{per}}(k,c)$ it follows by the formula

$$P_{\text{per}}(k,c) = \int_{\Lambda_{\text{per}}(k)} \mathrm{d}\zeta R_{\text{per}}(\zeta + c^2, k, c)$$

and proposition 4.2 that

$$\begin{aligned} P_{\text{per}}(k,c) &= \sum_{n=0}^{\infty} \frac{1}{c^n} \left(\int_{\Lambda_{\text{per}}(k)} \mathrm{d}\zeta R_{\text{per},n}(\zeta + c^2, k) \right) \\ &=: \sum_{n=0}^{\infty} \frac{1}{c^n} P_{\text{per},n}(k) \end{aligned}$$

where the power series is for all $m \in \mathbb{N}$ absolutely convergent in

$$\sup_{|\alpha| \le m} \sup_{k \in M^*} \|\partial_k^\alpha \cdot\|_{\mathcal{L}(\mathcal{H}_f, \mathcal{D})}$$

for $\frac{1}{c} \le R$. For $U_{\text{per}}(k,c)$ we know that

$$U_{\text{per},0} := U_{\text{per}}^P(k) \otimes \exp(iky) \tag{4.5}$$

is smooth, right τ-covariant and intertwines $P_{\text{per},0}(k)$ and $P_{\text{per},0}(0)$, i.e.

$$U_{\text{per},0}^*(k) P_{\text{per},0}(k) U_{\text{per},0}(k) = P_{\text{per},0}(0), \quad k \in M^*.$$

Now if we choose (w.l.o.g.) R small enough such that

$$\sup_{k \in M^*} \|P_{\text{per},0}(k) - P_{\text{per}}(k,c)\| < \frac{1}{2}$$

for all $\frac{1}{c} \le R$, we can define $U_{\text{per}}(k,c)$ using the Nagy formula, i.e.

$$\begin{aligned} &U_{\text{per}}(k,c) \\ &= \left(\mathbf{1} - (P_{\text{per},0}(k) - P_{\text{per}}(k,c))^2\right)^{-\frac{1}{2}} \\ &\quad \times \left(P_{\text{per},c}(k) P_{\text{per}}(k,c) + (\mathbf{1} - P_{\text{per},c}(k))(\mathbf{1} - P_{\text{per}}(k,c))\right). \end{aligned} \tag{4.6}$$

Now we know that

$$U_{\text{per}}^*(k,c) P_{\text{per}}(k,c) U_{\text{per}}(k,c) = P_{\text{per},0}(0).$$

Furthermore, by construction it is clear that $U_{\mathrm{per}}(k,c)$ is right τ-covariant and smooth in k. Furthermore, formula (4.6) shows that

$$U_{\mathrm{per}}(k,c) = \sum_{n=0}^{\infty} \frac{1}{c^n} U_{\mathrm{per},n}(k) \tag{4.7}$$

where the power series is for all $m \in \mathbb{N}$ absolutely convergent in

$$\sup_{|\alpha|\leq m} \sup_{k\in M^*} \|\partial_k^\alpha \cdot\|_{\mathcal{L}(\mathcal{H}_f,\mathcal{D})}$$

for $\frac{1}{c} \leq R$ and with $U_{\mathrm{per},0}(k)$ given in (4.5).

4.2 Adiabatic perturbation theory

Now we turn to the question how the results of the last section can be used to derive power series expansions of the symbols derived in section 2.2 resp. their quantizations. The following theorem follows from proposition 4.5 and the proof at the end of this section.

Theorem 4.4 *Let $\{E_n^P(k)\}_{n\in\mathcal{I}}$ be an isolated family of bands of the Pauli Hamiltonian and, for $\frac{1}{c} \leq R$, $\{E_n(k,c)\}_{n\in\mathcal{I}}$ be the corresponding isolated family $H_{per}(k,c)$ (see corollary 4.3). Then the following holds:*

1. *$\Pi_Z^{\varepsilon,c}, U^{\varepsilon,c}$ and $\widehat{h}(c)$ as in theorem 2.6 have power series expansions*

$$\Pi_Z^{\varepsilon,c} = \sum_{n=0}^{\infty} \frac{1}{c^n} \Pi_{Z,n}^{\varepsilon}, \quad U^{\varepsilon,c} = \sum_{n=0}^{\infty} \frac{1}{c^n} U_n^{\varepsilon} \text{ and } \widehat{h}(c) = \sum_{n=0}^{\infty} \frac{1}{c^{2n}} \widehat{h}_{2n}$$

   that converge absolutely and uniformly in ε for $\frac{1}{c} \leq R$.

2. *One has*

$$\|[\exp(-iH_Z^{\varepsilon,c}t), \Pi_Z^{\varepsilon,c}]\| = \mathcal{O}(c\varepsilon^\infty(1+|t|))$$

   and

$$\left\|\exp(-iH_Z^{\varepsilon,c}t)\Pi_Z^{\varepsilon,c} - (U^{\varepsilon,c})^* \left(\exp(-i\widehat{\mathbf{h}}(c)t) \oplus \mathbf{0}\right) U^{\varepsilon,c}\right\| = \mathcal{O}(c\varepsilon^\infty(1+|t|)).$$

To prove theorem 4.4 we start, as in section 4.1 with the Moyal resolvent $R(\zeta,c)$ and continue with studying the symbols $\pi(c)$, $u(c)$ and $h(c)$.

Proposition 4.5 *Let $\frac{1}{c} \leq R$ and $R_j(\zeta, c)$ be as constructed in lemma 2.10. Then there are coefficients $R_{j,n} \in S^{\mathbf{1}}_\tau(\mathcal{L}(\mathcal{H}_f))$, $j, n \in \mathbb{N}_0$ such that*

$$R_j(\zeta + c^2, c) = \sum_{n=0}^{\infty} \frac{1}{c^n} R_{j,n}(\zeta) \tag{4.8}$$

where the right hand side is, for any $m \in \mathbb{N}$, absolutely convergent in $\|\cdot\|^{(\mathbf{1})}_m$ uniformly in ζ. Furthermore, $R_{j,n}$ is diagonal resp. off-diagonal in the π_+-splitting for n even resp. odd and $R_{j,0} = \pi_+ R_{j,0} \pi_+$ for all $j \in \mathbb{N}_0$.

Proof. For R_0 we have immediately by proposition 4.2 that

$$R_0(\zeta + c^2, c, q, p) = \sum_{n=0}^{\infty} \frac{1}{c^n} R_{\text{per},n}(\zeta - \phi(p), q - A(p))$$

with convergence in $\|\cdot\|^{(\mathbf{1})}_m$ uniformly in ζ. Now assume that (4.8) is valid for $j \leq n$ and that furthermore for $j \leq n$

$$R_{j,0}(\zeta) = \pi_+ R_{j,0}(\zeta) \pi_+$$

and that $R_{j,l}$ is diagonal (resp. off-diagonal) in the π_+ splitting for l even (resp. odd) which is obviously satisfied for $j = 0$ (see also Thaller [Th]). Then for $n+1$ we have by definition

$$\begin{aligned} & R_{n+1}(\zeta + c^2, c) && (4.9) \\ = \;& -R_0(\zeta + c^2, c) \left(\left(H(c) - \zeta - c^2\right) \sharp \sum_{j \leq n} \varepsilon^j R_j(\zeta + c^2, c) \right)_{n+1} \\ = \;& -R_0(\zeta + c^2, c) \left((c\widetilde{q} \cdot \alpha + \phi \mathbf{1}) \sharp \sum_{j \leq n} \varepsilon^j R_j(\zeta + c^2, c) \right)_{n+1} \end{aligned}$$

where we used that the (q,p)-independent terms of $H(c,q,p)$ do not contribute to the right hand side. Obviously, we have

$$R_{n+1}(\zeta + c^2, c) =: c R_{j,-1}(\zeta) + \sum_{n=0}^{\infty} \frac{1}{c^n} R_{j,n}(\zeta)$$

where the power series part is for all $m \in \mathbb{N}$ absolutely convergent in $\|\cdot\|^{(\mathbf{1})}_m$ uniformly in ζ. Furthermore, from (4.9) it follows that all $R_{j,n}$ with n even (resp.

odd) are diagonal (resp. off-diagonal) because $c\alpha$ maps diagonal terms into off-diagonal terms (and vice versa) and shifts the index about 1 whereas $\phi(p)\mathbf{1}$ leaves diagonality resp. off-diagonality invariant. Finally we observe that

$$\begin{aligned} R_{n+1,-1}(\zeta) &= -R_{0,0}(\zeta)\left(c\widetilde{q}\cdot\alpha\sharp\sum_{j\leq n}\varepsilon^j R_{j,0}(\zeta)\right)_{n+1} \\ &= -\pi_+ R_{0,0}(\zeta)\left(c\widetilde{q}\cdot\pi_+\alpha\pi_+\sharp\sum_{j\leq n}\varepsilon^j R_{j,0}(\zeta)\pi_+\right)_{n+1} \\ &= 0 \end{aligned}$$

and

$$\begin{aligned} R_{n+1,0}(\zeta) &= -R_{0,0}(\zeta)\left(c\widetilde{q}\cdot\alpha\sharp\sum_{j\leq n}\varepsilon^j R_{j,1}(\zeta)\right)_{n+1} \\ &\quad -R_{0,1}(\zeta)\left(c\widetilde{q}\cdot\alpha\sharp\sum_{j\leq n}\varepsilon^j R_{j,0}(\zeta)\right)_{n+1} \\ &\quad -R_{0,0}(\zeta)\left(\phi\mathbf{1}\sharp\sum_{j\leq n}\varepsilon^j R_{j,1}(\zeta)\right)_{n+1} \\ &= \pi_+ R_{n+1,0}(\zeta)\pi_+ \end{aligned}$$

where we used that π_+ commutes with diagonal terms. ∎

Using proposition 4.5 we can expand the other symbols of chapter 2.

Proposition 4.6 *Let $\frac{1}{c}\leq R$ and $\pi_j(c)$, $u_j(c)$ and $\mathbf{h}_j(c)$ be as constructed in chapter 2. Then one has*

$$\pi_j(c)=\sum_{n=0}^{\infty}\frac{1}{c^n}\pi_{j,n},\ u_j(c)=\sum_{n=0}^{\infty}\frac{1}{c^n}u_{j,n}\ \text{and}\ \left(\mathbf{h}(c)-c^2\right)_j=\sum_{n=0}^{\infty}\frac{1}{c^{2n}}h_{j,2n}.$$

where the power series are, for any $m\in\mathbb{N}$, absolutely convergent in $\|\cdot\|_m^{(\mathbf{1})}$. For $j=0,1$, the zeroth order terms in $\frac{1}{c}$ are diagonal in the π_+-splitting and agree with the corresponding terms in the Pauli case of chapter 3, i.e.

$$\pi_{j,0}=\pi_j^P\otimes\mathbf{0},\ \pi_+u_{j,0}\pi_+=u_j^P\otimes\mathbf{0}\ \text{and}\ h_{j,0}=h_j^P\otimes\mathbf{0},\quad j=0,1.$$

In the case of a single eigenvalue of the Pauli Hamiltonian, i.e. $|\mathcal{I}|=2$ we have

$$(\mathbf{h}_{0,2})_{\nu,\mu}=\frac{1}{4}\left\langle\varphi_\nu^P,[-\frac{1}{2}\Delta_y^2-i\boldsymbol{\sigma}\cdot(\nabla V_\Gamma\times\nabla_y)+\frac{1}{2}\Delta V_\Gamma]\varphi_\mu^P\right\rangle,\quad \nu,\mu\in\mathcal{I}.$$

Proof. The definition

$$\begin{aligned}\pi_j(c) &= \int_{\Lambda^P+c^2} \mathrm{d}\zeta R_j(\zeta,c) \\ &= \int_{\Lambda^P} \mathrm{d}\zeta R_j(\zeta+c^2,c)\end{aligned}$$

gives the expansion

$$\pi_j(c) = \sum_{n=0}^{\infty} \frac{1}{c^n}\pi_{j,n}$$

where the right hand sides are, for any $m \in \mathbb{N}$, absolutely convergent in $\|\cdot\|_m^{(\mathbf{1})}$ for $\frac{1}{c} \leq R$. Next it follows that also the Moyal unitary u has a power series expansion

$$u_j(c) = \sum_{n=0}^{\infty} \frac{1}{c^n} u_{j,n}$$

absolutely convergent in $\|\cdot\|_m^{(\mathbf{1})}$ for all $m \in \mathbb{N}$ since u is constructed as a sum of products of $U^c_{\mathrm{per}}(q - A(p))$, π and their derivatives.

It remains to prove the statement about $\mathbf{h}$. We start with the observation that

$$\begin{aligned}H(c)\sharp\pi(c) &= \int_{\Lambda^P+c^2} \mathrm{d}\zeta R(\zeta,c)\zeta \\ &= \int_{\Lambda^P} \mathrm{d}\zeta R(\zeta+c^2,c)\zeta \\ &\quad + c^2\int_{\Lambda^P} \mathrm{d}\zeta R(\zeta+c^2,c) \\ &= \int_{\Lambda^P} \mathrm{d}\zeta R(\zeta+c^2,c)\zeta + c^2\pi(c).\end{aligned}$$

By the definition

$$\mathbf{h} \oplus \mathbf{0}_{\mathcal{K}_f^\perp} = u\sharp H\sharp\pi\sharp u^*$$

it follows that

$$\big(\mathbf{h}(c) - c^2\big)_j = \sum_{n=0}^{\infty} \frac{1}{c^n}\mathbf{h}_{j,n}$$

where the right hand side is absolutely convergent in $\|\cdot\|_m^{(\mathbf{1})}$ for all $m \in \mathbb{N}$. Next, we want to show that all odd coefficients $h_{j,2n+1}$ vanish. In the series expansion of $R_{\mathrm{per}}(\zeta+c^2,k,c)$, the odd coefficients are all off-diagonal in the π_+-splitting whereas the even coefficients are diagonal. The same holds true for $H_{\text{per}}(c)$. Since R, π, u and h are all constructed by multiplication, integration and differentiation of these quantities and the product of a diagonal term with a off-diagonal term gives an off-diagonal term whereas diagonal times diagonal terms and off-diagonal times off-diagonal terms give diagonal terms, we conclude that also in the expansion of $(\mathbf{h}(c) - c^2) \oplus \mathbf{0}_{\mathcal{K}_f^\perp}$ all odd coefficients are off-diagonal. However, we have that $\pi_r = \pi_+ \pi_r \pi_+$ and therefore all coefficients of $(\mathbf{h}(c) - c^2) \oplus \mathbf{0}_{\mathcal{K}_f^\perp}$ must be diagonal, therefore the odd ones must vanish.

To compute the zeroth order terms in $\frac{1}{c}$ explicitly, we state that since $R_{0,0}(\zeta) = R_0^P(\zeta) \otimes \mathbf{0}$ it follows that

$$\begin{aligned} \pi_{0,0} &= \int_\Lambda \mathrm{d}\zeta R_{0,0}(\zeta) \\ &= \pi_0^P \otimes \mathbf{0}. \end{aligned}$$

Furthermore, one has (see definition 4.5)

$$\begin{aligned} u_{0,0}\pi_+ &= U_{\text{per}}^{(0)}(q - A(p))\pi_+ \\ &= U_{\text{per}}^P(q - A(p)) \otimes \mathbf{0} \\ &= u_0^P \otimes \mathbf{0} \end{aligned}$$

and therefore

$$\mathbf{h}_{0,0} = \mathbf{h}_0^P.$$

Next, we turn to the first order terms, starting with the computation of $R_1(\zeta + c^2, c)$:

$$\begin{aligned} R_1(\zeta + c^2, c) &= -\left(R_0(\zeta + c^2, c) \sharp (H_0 - \zeta - c^2)\right)_1 R_0(\zeta + c^2, c) \\ &= \frac{i}{2}\{R_0(\zeta + c^2, c), H_0\} R_0(\zeta + c^2, c) \\ &= \frac{i}{2}\{R_{0,0}(\zeta), \phi\} R_{0,0}(\zeta) - \frac{i}{2}\{R_{0,1}(\zeta), \alpha \cdot \widetilde{q}\} R_{0,0}(\zeta) \\ &\quad -\frac{i}{2}\{R_{0,0}(\zeta), \alpha \cdot \widetilde{q}\} R_{0,1}(\zeta) + \mathcal{O}(\frac{1}{c}). \end{aligned}$$

Since the first term agrees with the corresponding term in the Pauli case, we go on with studying the second and third term.

For the second term we obtain, using the relation $(a\cdot\alpha)(b\cdot\alpha) = (a\cdot b)\,\mathbf{1} + i(a\times b)\cdot\mathbf{S}$ (and therefore $[a\cdot\alpha, b\cdot\alpha] = 2i(a\times b)\cdot\mathbf{S}$)

$$\begin{aligned}
&\frac{i}{2}\{R_{0,1}(\zeta), \boldsymbol{\alpha}\cdot\widetilde{q}\}R_{0,0}(\zeta)\\
&= \frac{i}{4}\{R_{0,0}(\zeta)(-i\nabla_y - \widetilde{q})\cdot\boldsymbol{\alpha}, \boldsymbol{\alpha}\cdot\widetilde{q}\}R_{0,0}(\zeta)\\
&\quad \underbrace{+\frac{i}{4}\{((-i\nabla_y - \widetilde{q})\cdot\boldsymbol{\alpha})\,R_{0,0}(\zeta), \boldsymbol{\alpha}\cdot\widetilde{q}\}R_{0,0}(\zeta)}_{=0}\\
&= -\frac{i}{4}R_{0,0}(\zeta)\{\widetilde{q}\cdot\boldsymbol{\alpha}, \boldsymbol{\alpha}\cdot\widetilde{q}\}R_{0,0}(\zeta)\\
&\quad +\frac{i}{4}\left(\{R_{0,0}(\zeta), \widetilde{q}\}\cdot(-i\nabla_y - \widetilde{q})\right)R_{0,0}(\zeta)\\
&\quad -\frac{1}{4}\left(\{R_{0,0}(\zeta), \widetilde{q}\}\times(-i\nabla_y - \widetilde{q})\right)\cdot\mathbf{S}R_{0,0}(\zeta).
\end{aligned}$$

The third term becomes

$$\begin{aligned}
&\frac{i}{2}\{R_{0,0}(\zeta), \alpha\cdot\widetilde{q}\}R_{0,1}(\zeta)\\
&= \frac{i}{4}\{R_{0,0}(\zeta), \alpha\cdot\widetilde{q}\}(-i\nabla_y - \widetilde{q})\cdot\boldsymbol{\alpha}R_{0,0}(\zeta)\\
&= \frac{i}{4}\{R_{0,0}(\zeta), \widetilde{q}\}\cdot(-i\nabla_y - \widetilde{q})R_{0,0}(\zeta)\\
&\quad +\frac{i}{4}\left(\{R_{0,0}(\zeta), \widetilde{q}\}\times(-i\nabla_y - \widetilde{q})\right)\cdot\mathbf{S}R_{0,0}(\zeta).
\end{aligned}$$

Putting this together, we arrive at

$$\begin{aligned}
R_{1,0}(\zeta) &= \frac{i}{2}\{R_{0,0}(\zeta), \phi\}R_{0,0}(\zeta) - \frac{i}{2}\left(\{R_{0,0}(\zeta), \widetilde{q}\}\cdot(-i\nabla_y - \widetilde{q})\right)R_{0,0}(\zeta)\\
&\quad +\frac{i}{4}R_{0,0}(\zeta)\{\widetilde{q}\cdot\boldsymbol{\alpha}, \boldsymbol{\alpha}\cdot\widetilde{q}\}R_{0,0}(\zeta)\\
&= \frac{i}{2}\{R_{0,0}(\zeta), (-i\nabla_y - \widetilde{q})^2 + \phi\}R_{0,0}(\zeta) + \frac{i}{2}\left(B(p)\cdot\mathbf{S}\right)R_{0,0}(\zeta)R_{0,0}(\zeta)\\
&= R_1^P(\zeta)\otimes\mathbf{0}.
\end{aligned}$$

Now it follows that

$$\begin{aligned}
\pi_{1,0} &= \pi_1^P\otimes\mathbf{0},\\
(H\sharp\pi)_{1,0} &= \int_{\Lambda_{\mathrm{per}}}\mathrm{d}\zeta\,\left(R_1^P(\zeta)\otimes\mathbf{0}\right)\zeta\\
&= (H^P\sharp\pi^P)_1\otimes\mathbf{0}
\end{aligned}$$

and also

$$u_{1,0}\pi_+ = u_1^P \otimes \mathbf{0}$$

since u_1 is constructed from u_0, π_0 and π_1.Now

$$\mathbf{h}_{1,0} = \mathbf{h}_1^P \otimes \mathbf{0}$$

follows directly.

In the case of a single eigenvalue band E_*^P, we can also compute the term of order $\frac{1}{c^2}$ in $\mathbf{h}_0$ as in [Th]: One has

$$\begin{aligned} & U_{\text{per}}\left(\int_{\Lambda_{\text{per}}} \mathrm{d}\zeta R_{\text{per}}(\zeta + c^2, k, c)\zeta\right) U_{\text{per}}^* \\ = \; & U_{\text{per}}\left(\int_{\Lambda_{\text{per}}} \mathrm{d}\zeta R_{\text{per}}(\zeta + c^2, k, c)(\zeta - E_*)\right) U_{\text{per}}^* + E_*\pi_r \\ = \; & \frac{1}{c^2} U_{\text{per}}\left(\int_{\Lambda_{\text{per}}} \mathrm{d}\zeta R_{\text{per},2}(\zeta, k)(\zeta - E_*)\right) U_{\text{per}}^* + E_*\pi_r + \mathcal{O}(\frac{1}{c^4}) \\ = \; & E_*^P\pi_r + \frac{1}{4c^2}\pi_r\left((-i\nabla_y + k)\cdot\boldsymbol{\sigma}\right)(V - E_*)\left((-i\nabla_y + k)\cdot\boldsymbol{\sigma}\right)\pi_r, \end{aligned}$$

where the terms $\int_{\Lambda_{\text{per}}} \mathrm{d}\zeta R_{\text{per},j}(\zeta, k)(\zeta - E_*)$ vanish for $j = 0, 1$ because $R_{\text{per},j}(\zeta, k)$ have only a pole of order 1 in E_*^P. Furthermore, if one knows that also the eigenvalue bands of $H_{\text{per}}(k)$ consist of a single eigenvalue E_* (e.g. in the case of inversion-symmetric V_Γ), one has furthermore that (again as in Thaller, p.188/189)

$$(\mathbf{h}_{0,2})_{\nu,\mu} = \frac{1}{4}\left\langle \varphi_\nu^P, [-\frac{1}{2}\Delta_y^2 - i\boldsymbol{\sigma}\cdot(\nabla V_\Gamma \times \nabla_y) + \frac{1}{2}\Delta V_\Gamma]\varphi_\mu^P \right\rangle, \quad \nu, \mu \in \mathcal{I}.$$

■

Now we are able to give the proof of theorem 4.4.

Proof. (of theorem 4.4) We first study how the resummation procedure of proposition A.7 can be adapted to the c-dependent case. Since the resummation is a subtle point, we introduce the notation $\widetilde{\pi}(c) = \sum_{j=0}^{N(\varepsilon)} \varepsilon^j \pi_j(c)$ etc. for the resummation in contrast to chapter 2 where we used π for both the formal power series and its resummation. For any formal symbol with coefficients π_j that have a power series expansion

$$\pi_j(c) = \sum_{n=0}^{\infty} \frac{1}{c^n}\pi_{j,n}$$

that is absolutely convergent in $\|\cdot\|_k^{(w)}$ for all $k \in \mathbb{N}$ for $\frac{1}{c} \leq R$, we replace in the proof of A.7 the definition

$$\varepsilon_k := \min\left(\frac{1}{k}, \frac{1}{2}\left(1 + \max_{l \leq k} \|\pi_l\|_k^{(w)}\right)^{-1}\right), \quad k \in \mathbb{N}$$

by

$$\varepsilon_k := \min\left(\frac{1}{k}, \frac{1}{2}\left(1 + \max_{l \leq k} \sup_{\frac{1}{c} \leq R} \sum_{n=0}^{\infty} \frac{1}{c^n} \|\pi_{l,n}\|_k^{(w)}\right)^{-1}\right), \quad k \in \mathbb{N}. \tag{4.10}$$

With this definition of ε_k, we construct resummations

$$\widetilde{\pi}(c) := \sum_{j=0}^{N(\varepsilon)} \varepsilon^j \pi_j(c)$$

and analogous for $\widetilde{u}, \widetilde{\mathbf{h}}$. Introducing $\widetilde{\pi}_n := \sum_{j=0}^{N(\varepsilon)} \varepsilon^j \pi_{j,n}$ etc. and the corresponding quantizations $\widehat{\pi}_n$ etc. we know that

$$\widehat{\pi}(c) = \sum_{n=0}^{\infty} \frac{1}{c^n} \widehat{\pi}_n, \ \widehat{u}(c) = \sum_{n=0}^{\infty} \frac{1}{c^n} \widehat{u}_n \text{ and } \widehat{\mathbf{h}}(c) - c^2 = \sum_{n=0}^{\infty} \frac{1}{c^{2n}} \widehat{h}_{2n} \tag{4.11}$$

where the right hand sides are absolutely convergent in $\sup_{\varepsilon \in [0,\varepsilon_0)} \|\cdot\|_{\mathcal{L}(\mathcal{H}_f)}$ resp. $\sup_{\varepsilon \in [0,\varepsilon_0)} \|\cdot\|_{\mathcal{L}(\mathcal{H}_f,\mathcal{H}_r)}$ resp $\sup_{\varepsilon \in [0,\varepsilon_0)} \|\cdot\|_{\mathcal{L}(\mathcal{H}_r)}$ because of definition 4.10. In order to not confuse $\widehat{\pi}_n$ as used in (4.11) with $\widehat{\pi_j}$, i.e. the quantization of the j-th coefficient of the formal power series π, we use in the following the expression $\widehat{\pi}(\infty) := \widehat{\pi}_0$, $\widetilde{\pi}(\infty) = \widetilde{\pi}_0$ etc.

We turn to the question how we can translate the results to $\Pi_Z^{\varepsilon,c}$ and $U^{\varepsilon,c}$. We know that with the explicit bounds of propositions A.7 and A.9

$$\left\|\widehat{\pi}^2(c) - \widehat{\pi}(c)\right\| = \mathcal{O}(\varepsilon^\infty)$$

uniformly in c because all $\|\pi_j\|_m^{(\mathbf{1})}$ are bounded uniformly in c. In particular,

$$\Pi_Z^{\varepsilon,c} = \int_{|\zeta - 1| = \frac{1}{2}} \mathrm{d}\zeta (\widehat{\pi}(c) - \zeta)^{-1}$$

is well-defined (for ε small enough independent of c) and

$$\Pi_Z^{\varepsilon,c} - \widehat{\pi}(c) = \mathcal{O}(\varepsilon^\infty)$$

uniformly in c. Furthermore,

$$\Pi_Z^{\varepsilon,c} = \sum_{n=0}^{\infty} \frac{1}{c^n} \Pi_{Z,n}^{\varepsilon}$$

where the right hand side converges in the operator-norm uniformly in ε since $(\widehat{\pi}(c) - \zeta)^{-1}$ has a power series expansion that converges uniformly in ε and ζ. Since $U^{\varepsilon,c}$ is constructed from $\widehat{u}(c)$ and $\Pi_Z^{\varepsilon,c}$ by analytic operations, i.e. multiplication and taking the square root, one can similarly show that

$$U^{\varepsilon,c} = \sum_{n=0}^{\infty} \frac{1}{c^n} U_n^{\varepsilon}$$

where the right hand side converges uniformly in ε and

$$U^{\varepsilon,c} - \widehat{u}(c) = \mathcal{O}(\varepsilon^{\infty})$$

uniformly in c.

Next, we want to estimate

$$\|[\exp(-iH_Z^{\varepsilon,c}t), \Pi_Z^{\varepsilon,c}]\|$$

From the proof of theorem 2.6, one can see that all the estimates involved hold uniformly in c except for the estimate of

$$H_Z^{\varepsilon,c}\widehat{\pi}(c) - (H_Z^{\varepsilon,c}\widehat{\pi}(c))^*$$

due to the fact that $H_Z^{\varepsilon,c}$ is polynomial in c. We use

$$\widehat{\pi}(c) = \widehat{\pi}(\infty) + \frac{1}{c} \sum_{n=0}^{\infty} \frac{1}{c^n} \widehat{\pi}_{n+1}$$

as in (4.11) with

$$\widehat{\pi}(\infty) = \pi_+ \widehat{\pi}(\infty) \pi_+ .$$

With

$$H_Z^{\varepsilon,c} = c^2 \boldsymbol{\beta} + c(-i\nabla_y + k - A(\varepsilon\nabla_k^{\tau})) \cdot \boldsymbol{\alpha} + V_{\Gamma}(y) + \phi(\varepsilon\nabla_k^{\tau})$$

and

$$c^2 \boldsymbol{\beta} \widehat{\pi}(\infty) = c^2 \widehat{\pi}(\infty) = \left(c^2 \boldsymbol{\beta} \widehat{\pi}(\infty)\right)^*$$

it follows that

$$\begin{aligned}
&c^{-1}\left(H_Z^{\varepsilon,c}\widehat{\pi}(c) - (H_Z^{\varepsilon,c}\widehat{\pi}(c))^*\right)\\
&\quad = c^{-1}\left((H_Z^{\varepsilon,c} - c^2\boldsymbol{\beta})\widehat{\pi}(\infty) - \left((H_Z^{\varepsilon,c} - c^2\boldsymbol{\beta})\widehat{\pi}(\infty)\right)^*\right)\\
&\qquad + c^{-1}\left(H_Z^{\varepsilon,c}(\widehat{\pi}(c) - \widehat{\pi}(\infty)) - (H_Z^{\varepsilon,c}(\widehat{\pi}(c) - \widehat{\pi}(\infty))^*\right)\\
&\quad = \mathcal{O}(\varepsilon^n)
\end{aligned}$$

with $\mathcal{O}(\varepsilon^n)$ uniformly in c because $c^{-1}(H - c^2\boldsymbol{\beta})$, $c^{-2}H$ and $c(\widetilde{\pi}(c) - \widetilde{\pi}(\infty))$ are bounded uniformly in c. Finally we estimate

$$\begin{aligned}
&\exp(-iH_Z^{\varepsilon,c}t)\Pi_Z^{\varepsilon,c} - (U^{\varepsilon,c})^*\left(\exp(-i\widehat{\mathbf{h}}(c)t) \oplus \mathbf{0}\right)U^{\varepsilon,c}\\
&\quad = \exp(-i\left(H_Z^{\varepsilon,c} - c^2\mathbf{1}_{\mathcal{H}_f}\right)t)\Pi_Z^{\varepsilon,c}\\
&\qquad - (U^{\varepsilon,c})^*\left(\exp(-i\left(\widehat{\mathbf{h}}(c) - c^2\mathbf{1}_{\mathcal{K}}\right)t) \oplus \mathbf{0}_{\mathcal{K}^\perp}\right)U^{\varepsilon,c}
\end{aligned}$$

in a similar way. All the estimates done in the proof of theorem 2.6 are uniformly in c except for the estimate of

$$\begin{aligned}
&\left(H_Z^{\varepsilon,c}(c) - c^2\mathbf{1}_{\mathcal{H}_f}\right)\widehat{\pi}(c) - (U^{\varepsilon,c})^*\left(\widehat{\mathbf{h}}(c) - c^2\mathbf{1}_{\mathcal{K}}\right) \oplus \mathbf{0}_{\mathcal{K}^\perp}U^{\varepsilon,c}\\
&\quad = \left(H_Z^{\varepsilon,c} - c^2\boldsymbol{\beta}\right)\widehat{\pi}(\infty) + \left(H_Z^{\varepsilon,c} - c^2\mathbf{1}_{\mathcal{H}_f}\right)(\widehat{\pi}(c) - \widehat{\pi}(\infty))\\
&\qquad - (U^{\varepsilon,c})^*\left(\widehat{\mathbf{h}}(c) - c^2\mathbf{1}_{\mathcal{K}}\right) \oplus \mathbf{0}_{\mathcal{K}^\perp}U^{\varepsilon,c}
\end{aligned}$$

where we used that $\widehat{\pi}(\infty) = \pi_+\widehat{\pi}(\infty)\pi_+$. However, one has that $c^{-1}(H - c^2\boldsymbol{\beta})$, $c^{-2}\left(H_Z^{\varepsilon,c} - c^2\mathbf{1}_{\mathcal{H}_f}\right)$ and $c(\widehat{\pi}(c) - \widehat{\pi}(\infty))$ as well as their corresponding symbols are uniformly bounded in c, therefore the substitution of the Weyl-product $\widetilde{\sharp}$ with the Moyal product $\sharp$ costs an error of order $\mathcal{O}(c\varepsilon^\infty)$ which concludes the proof. ■

4.3 Semiclassical limit

The last step in our analysis of the nonrelativistic limit is to study the semiclassical limit. Combining the results of our previous theorems, we arrive at the following result.

Theorem 4.7 *Let E_* be an isolated two-fold degenerate Bloch band of the Pauli Hamiltonian and $\Phi^t_{\varepsilon,P}$ be the flow defined in (3.6) and (3.7). Let furthermore*

$b \in C_b^\infty(\mathbb{R}^6 \times S^2, \mathbb{C})$ be Γ^*-periodic in the second argument, i.e. $b(q, p+\gamma^*) = b(q,p)$, let $\Pi^{\varepsilon,c} := (\mathcal{U}^{-1} \otimes \mathbf{1}_{\mathbb{C}^4})\, \Pi_Z^{\varepsilon,c}\, (\mathcal{U} \otimes \mathbf{1}_{\mathbb{C}^4})$ and

$$\mathbf{b}_\varepsilon(t) := 2 \int_{S^2} d\lambda(n) b \circ \Phi^t_{\varepsilon,P}(\cdot,\cdot,n) \left(\frac{1}{2}\mathbf{1}_{\mathbb{C}^4} + \sqrt{\frac{3}{4}} n \cdot \mathbf{S} \right)$$

with $\mathbf{b}_\varepsilon := \mathbf{b}_\varepsilon(0)$. Then, for $\frac{1}{c} \le R$ one has

$$\Pi^{\varepsilon,c} \left(\exp(iH^{\varepsilon,c}t/\varepsilon)\widehat{\mathbf{b}} \exp(-iH^{\varepsilon,c}t/\varepsilon) - \widehat{\mathbf{b}_0(t)} \right) \Pi^{\varepsilon,c} = \mathcal{O}(c\varepsilon^\infty(1+|t|)) + \mathcal{O}(\frac{1}{c}) + \mathcal{O}(\varepsilon)$$

and, if b is independent of n,

$$\Pi^{\varepsilon,c} \left(\exp(iH^{\varepsilon,c}t/\varepsilon)\widehat{\mathbf{b}} \exp(-iH^{\varepsilon,c}t/\varepsilon) - \widehat{\mathbf{b}_\varepsilon(t)} \right) \Pi^{\varepsilon,c} = \mathcal{O}(c\varepsilon^\infty(1+|t|)) + \mathcal{O}(\frac{1}{c}) + \mathcal{O}(\varepsilon^2)$$

uniformly for any finite time interval, where the Weyl quantization is in the sense of $\widehat{\mathbf{b}} = \mathbf{b}(-i\nabla_x, \varepsilon x)$.

Proof. From theorem 2.6 it follows that

$$\left\| \exp(-iH_Z^{\varepsilon,c}t)\Pi_Z^{\varepsilon,c} - (U^{\varepsilon,c})^* \left(\exp(-i\widehat{\mathbf{h}}(c)t) \oplus \mathbf{0} \right) U^{\varepsilon,c} \right\| = \mathcal{O}(c\varepsilon^\infty(1+|t|)).$$

From proposition 4.6, it follows that h_j and u_j agree, for $j = 0, 1$ with the corresponding Pauli quantities up to order $\mathcal{O}(\frac{1}{c^2})$ resp. $\mathcal{O}(\frac{1}{c})$. Together with the construction of $U^{\varepsilon,P}$ in the proof of theorem 4.4, it follows that $U_Z^{\varepsilon,c}$ and $\widehat{\mathbf{h}}(c)$ agree with the corresponding Pauli quantities up to order $\mathcal{O}(\frac{1}{c} + \varepsilon^2)$, therefore

$$(U^{\varepsilon,c})^* \left(\exp(-i\widehat{\mathbf{h}}(c)t) \oplus \mathbf{0} \right) U^{\varepsilon,c} - \left((U_P^\varepsilon)^* \left(\exp(-i\widehat{\mathbf{h}}_P t) \oplus \mathbf{0} \right) U_P^\varepsilon \right) \otimes \mathbf{0}_{L^2_\tau(\mathbb{R}^3, L^2(\mathbb{T}^3)\otimes\mathbb{C}^2)}$$

is of order $\mathcal{O}(\frac{1}{c} + \varepsilon^2)$. Furthermore, from theorem 3.4 we have

$$\exp(-iH^\varepsilon_{Z,P}t)\Pi^\varepsilon_{Z,P} - U_P^{\varepsilon *} \left(\exp(-i\widehat{\mathbf{h}}_P t) \oplus \mathbf{0} \right) U_P^\varepsilon = \mathcal{O}(\varepsilon^\infty(1+|t|)).$$

Together we have

$$\begin{aligned} &\exp(-iH_Z^{\varepsilon,c}t)\Pi_Z^{\varepsilon,c} - \exp(-iH^\varepsilon_{Z,P}t)\Pi^\varepsilon_{Z,P} \otimes \mathbf{0}_{L^2_\tau(\mathbb{R}^3, L^2(\mathbb{T}^3)\otimes\mathbb{C}^2)} \\ &= \mathcal{O}(c\varepsilon^\infty(1+|t|)) + \mathcal{O}(\frac{1}{c}) + \mathcal{O}(\varepsilon^2). \end{aligned}$$

Now theorem 3.8 gives the desired result by observing that the translation to the physical representation is independent of c and does not affect the π_+-splitting. ∎

A Pseudodifferential calculus

In this appendix, we give a short overview on pseudodifferential calculus. For the proofs and also a detailed description, we refer to [Fo] and also the appendix of [Teu]. In the whole paragraph we assume that $\mathcal{H}_1$, $\mathcal{H}_2$ and $\mathcal{H}_3$ are separable Hilbert spaces. In the following, we use multiindices $\alpha \in \mathbb{N}_0^d$ and define, as usual $|\alpha| := \sum_{l=1}^{d} \alpha_l$ and $\alpha! := \prod_{l=1}^{d} \alpha_l!$.

A.1 Weyl quantization and symbol classes

The basic idea of quantization is to associate to a function on a phase space $\mathbb{R}^{2d}$ an operator on the Hilbert space $L^2(\mathbb{R}^d)$. One requires that the function $(q,p) \mapsto q$ is turned into multiplication with x and the function $(q,p) \mapsto p$ is turned into the differential operator $-i\varepsilon\nabla_x$ for some $\varepsilon > 0$. If one has a function of the type

$$f(q,p) = g(q) + h(p)$$

one can easily define a quantization rule because $g(-i\varepsilon\nabla_x)$ and $g(x)$ are defined via the functional calculus for operators on $L^2(\mathbb{R}^d)$. For more general functions, such an easy definition is not possible since $-i\varepsilon\nabla_x$ and x do not commute. A possible choice is the Weyl-quantization rule which is in some sense "symmetric" in (q,p) and has the advantage that it maps real-valued functions into self-adjoint operators. To define the Weyl quantization, let A be a $\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$-valued smooth and rapidly decreasing function, i.e. $A \in \mathcal{S}(\mathbb{R}^{2d}, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$. Then we can express A as

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

where $\mathcal{F}A$ denotes the Fourier transform of A. Now due to

$$L^2(\mathbb{R}^d, \mathcal{H}_1) \cong L^2(\mathbb{R}^d) \otimes \mathcal{H}_1$$

it seems reasonable to replace in (A.1)

$$e^{i(\eta\cdot q + \xi\cdot p)} \mapsto e^{i(\eta\cdot \hat{q} + \xi\cdot \hat{p})} \otimes \mathbf{1}_{\mathcal{H}_1}$$

where $\widehat{q}$ is multiplication with x and $\widehat{p} = -i\varepsilon\nabla_x$. One arrives at the expression

$$\frac{1}{(2\pi)^d}\int_{\mathbb{R}^{2d}} \mathrm{d}\eta \mathrm{d}\xi e^{i(\eta\cdot\hat{q}+\xi\cdot\hat{p})} \otimes (\mathcal{F}A)(\eta,\xi). \tag{A.2}$$

For $\psi \in L^2(\mathbb{R}^d)$, the exponential is explicitly given by

$$\left(e^{i(\eta\cdot\hat{q}+\xi\cdot\hat{p})}\psi\right)(x) = e^{i\varepsilon\frac{(\eta\cdot\xi)}{2}} e^{i\eta\cdot x}\psi(x+\varepsilon\xi), \tag{A.3}$$

therefore if $\mathcal{F}A$ belongs to $L^1(\mathbb{R}^{2d}, \mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$ then $\widehat{A} : L^2(\mathbb{R}^d,\mathcal{H}_1) \to L^2(\mathbb{R}^d,\mathcal{H}_2)$ given by

$$\widehat{A}\psi = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^{2d}} \mathrm{d}\eta \mathrm{d}\xi e^{i(\eta\cdot\hat{q}+\xi\cdot\hat{p})} \otimes (\mathcal{F}A)(\eta,\xi)\psi, \quad \psi \in L^2(\mathbb{R}^d,\mathcal{H}_1) \tag{A.4}$$

is a bounded operator with

$$\left\|\widehat{A}\right\|_{\mathcal{L}(L^2(\mathbb{R}^d,\mathcal{H}_1),L^2(\mathbb{R}^d,\mathcal{H}_2))} \le \frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^{2d}} \mathrm{d}\xi \mathrm{d}y \left\|(\mathcal{F}A)(\eta,\xi)\right\|_{\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)}.$$

If we put (A.3) into (A.2) then for $\psi \in \mathcal{S}(\mathbb{R}^d,\mathcal{H}_1)$ we have the explicit formula

$$\varphi(x) = \frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^{2d}} \mathrm{d}\xi \mathrm{d}y A(\frac{1}{2}(x+y),\xi) e^{\frac{i}{\varepsilon}\xi\cdot(x-y)}\psi(y). \tag{A.5}$$

where

$$\varphi = \left(\frac{1}{(2\pi)^d}\int_{\mathbb{R}^{2d}} \mathrm{d}\eta \mathrm{d}\xi e^{i(\eta\cdot\hat{q}+\xi\cdot\hat{p})} \otimes (\mathcal{F}A)(\eta,\xi)\right)\psi.$$

If $\psi \in \mathcal{S}(\mathbb{R}^d,\mathcal{H}_1)$ then the formula (A.5) makes sense not only for A with $\mathcal{F}A \in L^1(\mathbb{R}^{2d},\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$ but for a larger class of symbols. The type of symbol classes which we are going to use are defined in terms of so called order functions.

Definition A.1 *A function $w : \mathbb{R}^d \to (0,\infty)$ is called order function if there are positive constants C_0 and $N_0 \in \mathbb{N}$ such that*

$$w(x) \le C_0 \langle x-y\rangle^{N_0} w(y) \quad \forall x,y \in \mathbb{R}^d$$

where $\langle x\rangle := (1+|x|^2)^{\frac{1}{2}}$.

If w_1, w_2 are order functions, then so is $w_1 + w_2$ (obviously) and $w_1 \cdot w_2$ because

$$\begin{aligned} w_1\cdot w_2(x) &= w_1(x)\cdot w_2(x) \\ &\le C_0\langle x-y\rangle^{N_0} w_1(y) C_0'\langle x-y\rangle^{N_0'} w_2(y) \\ &= C_0C_0'\langle x-y\rangle^{N_0+N_0'} w_1(y)\cdot w_2(y). \end{aligned}$$

Furthermore, the function $\langle\cdot\rangle$ (hence also $\langle\cdot\rangle^n$, $n \in \mathbb{N}$) is an order function, whereas for each order function w with $w(x) \leq C_0 \langle x-y\rangle^{N_0} w(y) \quad \forall x, y \in \mathbb{R}^{2d}$, clearly we also have $w(x) \leq C_0 \langle x\rangle^{N_0} w(0)$ resp. $C_0 w(y) \geq \langle y\rangle^{-N_0} w(0)$ by setting $y = 0$ resp. $x = 0$. Now we have the ingredients to define our symbol classes.

Definition A.2 *Let w be an order function. Then we define*

$$\|A\|_k^{(w,\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))} := \max_{|\alpha|\leq k} \sup_{x\in\mathbb{R}^{2d}} \Big(\|(\partial^\alpha A)(x)\|_{\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)} w^{-1}(x) \Big)$$

for A in $\mathcal{C}^\infty(\mathbb{R}^{2d}, \mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$. The superscript $\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)$ is omitted in the following whenever no confusion arises. Furthermore we define

$$S^w(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)) := \{A \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)) : \|A\|_k^{(w)} < \infty \forall k \in \mathbb{N}_0\}$$

and

$$S(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)) := \bigcup_{w \text{ order function}} S^w(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)).$$

Remark A.3 *We state that $S^{w_1}(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)) \subseteq S^{w_2}(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$ if $w_1 \leq const \cdot w_2$. Furthermore $S(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$ is a complex vector space and $S^w(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$ are subspaces. Together with the directed family of norms*

$$\|\cdot\|_k^{(w,\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))}, \quad k \in \mathbb{N}_0$$

$S^w(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$ are Fréchet spaces.

Proposition A.4 *Let $A \in S^w(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$, then (A.5) defines a continuous mapping from $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_1)$ to $\mathcal{S}(\mathbb{R}^d, \mathcal{H}_2)$. More precisely (in the notation of (A.5)) there is a $m \in \mathbb{N}$ depending on w and d such that for all $n \in \mathbb{N}$*

$$\|\varphi\|_n^{\mathcal{S}} \leq C_{n,w} \|A\|_{n+m}^{(w)} \|\psi\|_{n+m}^{\mathcal{S}}$$

where

$$\|\psi\|_n^{\mathcal{S}} := \sup_{|\alpha|\leq n} \sup_{x\in\mathbb{R}^d} \|\langle x\rangle^n \partial^\alpha \psi(x)\|_{\mathcal{H}_i}, \quad i = 1, 2.$$

Proof. If $\psi \in \mathcal{S}(\mathbb{R}^d, \mathcal{H}_1)$, then clearly

$$g(x,\xi) = \int_{\mathbb{R}^d} \mathrm{d}y A(\frac{1}{2}(x+y),\xi)\psi(y)e^{-\frac{i}{\varepsilon}\xi\cdot y}$$

is well-defined and smooth. Moreover, the integrand is a Schwartz function for each x, ξ and we get by partial integration

$$g(x,\xi) = \int_{\mathbb{R}^d} \mathrm{d}y e^{-\frac{i}{\varepsilon}\xi\cdot y} \langle\xi\rangle^{-2M} (1-\varepsilon^2\Delta_y) A(\frac{1}{2}(x+y),\xi)\psi(y)$$

from which it follows that

$$|g(x,\xi)| \leq C_M \langle\xi\rangle^{-2M} w(\frac{1}{2}x,\xi) \|A\|^{(w)}_{2M} \left(\int_{\mathbb{R}^d} \mathrm{d}y \left\langle \frac{1}{2}y \right\rangle^{N_w} \sup_{|\alpha|\leq 2M} \|\partial^\alpha \psi(y)\| \right)$$

where we used $w(x) \leq C_w \langle y-x\rangle^{N_w} w(y)$. Since $w(x,\xi)$ is polynomially bounded in ξ, it follows that $g(x,\cdot)$ decays for fixed x faster that any polynomial, in particular

$$\varphi(x) = \frac{1}{(2\pi\varepsilon)^d} \int_{\mathbb{R}^{2d}} \mathrm{d}\xi e^{\frac{i}{\varepsilon}\xi\cdot x} g(x,\xi)$$

is well-defined. Again by partial integration one can show that

$$\begin{aligned} \left|\partial_x^\beta \partial_\xi^\alpha g(x,\xi)\right| &\leq C'_M \langle\xi\rangle^{-2M} w(\frac{1}{2}x,\xi) \|A\|^{(w)}_{2M+|\alpha|+|\beta|} \\ & \times \left(\int_{\mathbb{R}^d} \mathrm{d}y \left\langle \frac{1}{2}y \right\rangle^{|\alpha|+N_w} \sup_{|\alpha|\leq 2M} \|\partial^\alpha \psi(y)\| \right) \end{aligned}$$

and therefore $\partial_x^\beta g(x,\cdot)$ is even a Schwartz function. Now we are able to use partial integration also in the outer integral and arrive at

$$\begin{aligned} &\langle x\rangle^n \partial_x^\alpha \varphi(x) \\ &= \frac{1}{(2\pi\varepsilon)^d} \sum_{|\beta+\gamma|\leq|\alpha|} c_{\beta,\gamma} \int_{\mathbb{R}^{2d}} \mathrm{d}\xi \langle x\rangle^n \xi^\beta e^{\frac{i}{\varepsilon}\xi\cdot x} \partial_x^\gamma g(x,\xi) \\ &\quad \frac{1}{(2\pi\varepsilon)^d} \sum_{|\beta+\gamma|\leq|\alpha|} c_{\beta,\gamma} \int_{\mathbb{R}^{2d}} \mathrm{d}\xi \langle x\rangle^{-2N+n} e^{\frac{i}{\varepsilon}\xi\cdot x} (1-\varepsilon^2\Delta_\xi)^N \xi^\beta \partial_x^\gamma g(x,\xi). \end{aligned}$$

Choosing M, N large enough one has that φ is indeed a Schwartz function and moreover that its Schwartz norms can be bounded by the $\|\cdot\|^{(w)}$-norms of A and the Schwartz norms of ψ. ■

Whereas (A.2) was only a formal expression, we can now define

$$\mathcal{W}_\varepsilon^{\mathcal{S}}(A) : \mathcal{S}(\mathbb{R}^d,\mathcal{H}_1) \to \mathcal{S}(\mathbb{R}^d,\mathcal{H}_2), \quad A \in S(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$$

through (A.5). By duality one can extend $\mathcal{W}_\varepsilon^{\mathcal{S}}(A)$ to a continuous mapping

$$\mathcal{W}_\varepsilon^{\mathcal{S}'}(A) : \mathcal{S}'(\mathbb{R}^d, \mathcal{H}_1) \to \mathcal{S}'(\mathbb{R}^d, \mathcal{H}_2).$$

More precisely, we choose the (anti-linear) inclusions

$$\mathcal{S}(\mathbb{R}^d, \mathcal{H}_i) \ni \psi \mapsto T_\psi \in \mathcal{S}'(\mathbb{R}^d, \mathcal{H}_i), \quad i = 1, 2$$

with

$$T_\psi(\varphi) = \int_{\mathbb{R}^d} \mathrm{d}x \, \langle \psi(x), \varphi(x) \rangle_{\mathcal{H}_i}$$

and define

$$\left[\left(\mathcal{W}_\varepsilon^{\mathcal{S}'}(A)\right)(T)\right](\varphi) = T\left[\left(\mathcal{W}_\varepsilon^{\mathcal{S}'}(A^*)\right)(\varphi)\right].$$

Note that taking the pointwise adjoint of A does not affect the symbol class. An important fact in pseudodifferential calculus is, that symbols in $S^{w=\mathbf{1}}(\mathcal{L}(\mathcal{H}))$ become bounded operators on $L^2(\mathbb{R}^d, \mathcal{H})$:

Proposition A.5 (Calderon-Vaillancourt) *There is a constant $C_d < \infty$ such that for every $A \in S^{\mathbf{1}}(\mathcal{L}(\mathcal{H}))$, $\mathcal{W}_\varepsilon^{\mathcal{S}'}(A)$ can be restricted to a bounded operator*

$$\widehat{A} = \mathcal{W}_\varepsilon^{L^2}(A) \in \mathcal{L}(L^2(\mathbb{R}^d, \mathcal{H}))$$

with

$$\left\|\widehat{A}\right\|_{\mathcal{L}(L^2(\mathbb{R}^d, \mathcal{H}))} \leq C_d \, \|A\|_{2d+1}^{(\mathbf{1})}.$$

For the proof see Theorem 2.73 in [Fo]. This theorem is in particular useful to translate estimates about the symbols into statements about the corresponding operators. We note furthermore that if $A \in S^{\mathbf{1}}(\mathcal{L}(\mathcal{H}))$ is pointwise self-adjoint, then $\widehat{A}$ is a self-adjoint operator on $L^2(\mathbb{R}^d, \mathcal{H})$.

Since the Weyl-product $\widetilde{\sharp}_\varepsilon$, that is introduced in the next section, can be formally expanded in powers of ε, it makes sense to define suitable classes of ε-dependent symbols, the so-called semiclassical symbols.

Definition A.6 *A map $a : (0, \varepsilon_0) \to S^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$, $\varepsilon \mapsto a_\varepsilon$ is a semiclassical symbol with order function w if there is a sequence $\{A_j\}_{j \in \mathbb{N}}$ with $A_j \in S^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ such that for every $n \in \mathbb{N}$ one has that*

$$\sup_{\varepsilon \in (0, \varepsilon_0)} \left\| a_\varepsilon - \sum_{j=0}^{n} \varepsilon^j A_j \right\|_l^{(w)} \varepsilon^{-(n+1)} < \infty.$$

If this is the case, we write

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

The space of these symbols is denoted by $S^w(\varepsilon_0, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ *or short as* $S^w(\varepsilon_0)$ *if clear from the context. Furthermore*

$$S(\varepsilon_0) := \bigcup_{w \text{ order function}} S^w(\varepsilon_0)$$

In this context it is also convenient to introduce the space of formal power series with coefficients in $S^w(\varepsilon_0, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ as

$$\begin{aligned} M^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)) \ &: = \{\sum_{j\geq 0} \varepsilon^j a_j : a_j \in S^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))\} \\ M(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)) \ &: = \bigcup_{w \text{ order function}} M^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)). \end{aligned}$$

Observe that it is not required for the formal power series to converge in any sense. However, every formal power series in $M^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ is the expansion of a (non-unique) semiclassical symbol as explained in detail in the following proposition (see also proposition 2.26 in [Fo]).

Proposition A.7 *Let* $\{A_j\}_{j\in\mathbb{N}}$ *be an arbitrary sequence in* $S^{(w)}(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$. *Then there is a* $a \in S^{(w)}(\varepsilon_0, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ *such that* $a_\varepsilon \asymp \sum_{j=0}^\infty \varepsilon^j A_j$ *in* $S^{(w)}(\varepsilon_0, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$. *Furthermore, a is unique up to a symbol that is* $\mathcal{O}(\varepsilon^\infty)$ *in* $\|\cdot\|_k^{(w)}$ *for any* $k \in \mathbb{N}$ *and uniformly in* ε. *The semiclassical symbol a is called a resummation of the formal symbol* $\sum_{j\geq 0} \varepsilon^j A_j$.

Proof. We define

$$\varepsilon_n := \min\left(\frac{1}{n}, \frac{1}{2}\left(1 + \max_{l\leq n} \|A_l\|_n^{(w)}\right)^{-1}\right), \quad n \in \mathbb{N}.$$

Note that $(\varepsilon_n)_{n\in\mathbb{N}}$ is monotone decreasing and converging against 0. We define furthermore $a : [0, \varepsilon_0) \to S^{(w)}(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ by

$$a_\varepsilon := \sum_{j=0}^{\infty} \varepsilon^j \mathbf{1}_{[0,\varepsilon_j)}(\varepsilon) A_j.$$

Then one has

$$
\begin{aligned}
&\sup_{\varepsilon\in[0,\varepsilon_0)} \varepsilon^{-(N+1)} \left\| a_\varepsilon - \sum_{j=0}^{N} \varepsilon^j A_j \right\|_k^{(w)} \\
= &\sup_{\varepsilon\in[0,\varepsilon_{N+1})} \varepsilon^{-(N+1)} \left\| \sum_{j=N+1}^{\infty} \varepsilon^j \mathbf{1}_{[0,\varepsilon_j)} A_j \right\|_k^{(w)} \\
&+ \sup_{\varepsilon\in[\varepsilon_N,\varepsilon_0)} \varepsilon^{-(N+1)} \left\| \sum_{j=0}^{N} \varepsilon^j \left(\mathbf{1}_{[0,\varepsilon_j)} - \mathbf{1}_{[0,\varepsilon_0)}\right) A_j \right\|_k^{(w)} \\
\leq &\sum_{j=0}^{\infty} \left\| \varepsilon_{j+N+1}^j A_{j+N+1} \right\|_k^{(w)} + \varepsilon_N^{-(N+1)} \varepsilon_0^N \max_{j\leq N} \|A_j\|_k^{(w)} \\
\leq &\sum_{j=0}^{\infty} \frac{1}{2^j} \left(1 + \max_{l\leq j+N+1} \|A_l\|_{j+N+1}^{(w)}\right)^{-j} \|A_{j+N+1}\|_k^{(w)} + \varepsilon_N^{-(N+1)} \varepsilon_0^N \max_{j\leq N} \|A_j\|_k^{(w)} \\
\leq &\sum_{j=0}^{\max(0,k-N-2)} \frac{1}{2^j} \|A_{j+N+1}\|_k^{(w)} + \sum_{j=\max(0,k-N-2)+1}^{\infty} \frac{1}{2^j} + \varepsilon_N^{-(N+1)} \varepsilon_0^N \max_{j\leq N} \|A_j\|_k^{(w)} \\
\leq &\; 2 \max_{j\leq k} \|A_j\|_k^{(w)} + 2 + \varepsilon_N^{-(N+1)} \varepsilon_0^N \max_{j\leq N} \|A_j\|_k^{(w)} .
\end{aligned}
$$

The uniqueness statement follows by linearity because the difference of two resummations a, a' must have the zero series as expansion. ■

A.2 The Weyl-Moyal product

The most useful property of symbols is that one can define an associative product between symbols that corresponds to the composition of operators. To be more precise, we have the following proposition (see [Fo], theorem 2.47):

Proposition A.8 *Let* $A \in S^{w_1}(\mathcal{L}(\mathcal{H}_2, \mathcal{H}_3))$, $B \in S^{w_2}(\mathcal{L}(\mathcal{H}_2, \mathcal{H}_3))$. *Then*

$$\mathcal{W}_\varepsilon^{\mathcal{S}'}(A)\mathcal{W}_\varepsilon^{\mathcal{S}'}(B) = \mathcal{W}_\varepsilon^{\mathcal{S}'}(C)$$

with $C \in S^{w_1 w_2}(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_3))$ *given by*

$$\begin{aligned} C(q,p) &= \left(\frac{2}{\varepsilon\pi}\right)^d \int_{\mathbb{R}^{4d}} dq\prime dp\prime dq\prime\prime dp\prime\prime \exp(\frac{2i}{\varepsilon}(q-q\prime)^\top (p-p\prime\prime)) \\ &\quad \times \exp(-\frac{2i}{\varepsilon}(q-q\prime\prime)^\top (p-p\prime)) A(q\prime,p\prime) B(q\prime\prime,p\prime\prime) \\ &=: \left(A \widetilde{\sharp}_\varepsilon B\right)(q,p). \end{aligned} \tag{A.6}$$

Furthermore there is a $m \in \mathbb{N}$ *depending on* w *and* d *such that for all* $n \in \mathbb{N}$

$$\|C\|_n^{(w_1 w_2)} \leq C_{n,w} \|A\|_{n+m}^{(w_1)} \|B\|_{n+m}^{(w_2)}$$

Proof. The full proof is given in [Fo], we only sketch the idea. Note that a priori (A.6) is not necessarily well-defined for arbitrary A, B, but only e.g. for A, B with compact support. Therefore, it is part of the proof to show in which sense (A.6) is to be understood. To give a formal derivation of the formula, we note that by definition

$$\begin{aligned} &\left(\mathcal{W}_\varepsilon^{\mathcal{S}}(C)\psi\right)(x) \\ &= \frac{1}{(2\pi\varepsilon)^d} \int_{\mathbb{R}^d} \mathrm{d}z \left(\int_{\mathbb{R}^d} \mathrm{d}\xi'' C(\frac{1}{2}(x+z), \xi'') e^{\frac{i}{\varepsilon}\xi''\cdot(x-z)} \right) \psi(z) \\ &=: \frac{1}{(2\pi\varepsilon)^d} \int_{\mathbb{R}^d} \mathrm{d}z K_C(x,z)\psi(z). \end{aligned}$$

Furthermore, for $x, z \in \mathbb{R}^d$

$$
\begin{aligned}
&K_C(x,z)\\
&= \left(\frac{2}{\varepsilon\pi}\right)^d \int_{\mathbb{R}^d} \mathrm{d}\xi'' \exp(\frac{i}{\varepsilon}\xi'' \cdot (x-z))\\
&\quad \times \int_{\mathbb{R}^{4d}} \mathrm{d}q'\mathrm{d}p'\mathrm{d}q''\mathrm{d}p'' \exp(\frac{i}{\varepsilon}(x+z-2q')\cdot(\xi''-p''))\\
&\quad \times \exp(-\frac{i}{\varepsilon}(x+z-2q'')\cdot(\xi''-p'))A(q',p')B(q'',p'')\\
&= \left(\frac{2}{\varepsilon\pi}\right)^d \int_{\mathbb{R}^{3d}} \mathrm{d}p'\mathrm{d}q'\mathrm{d}p'' \exp(\frac{i}{\varepsilon}(x-z)\cdot p'')\\
&\quad \times \exp(\frac{2i}{\varepsilon}(q'-x)\cdot(p''-p'))A(q',p')\\
&\quad \times \int_{\mathbb{R}^d} \mathrm{d}\xi'' \exp(-\frac{i}{\varepsilon}\left(q' - \frac{1}{2}(x-z)\right)\cdot 2(\xi''-p'))\\
&\quad \times \int_{\mathbb{R}^d} \mathrm{d}q'' \exp(\frac{i}{\varepsilon}(q''\cdot 2(\xi''-p'))B(q'',p'')\\
&= \left(\frac{2}{\varepsilon\pi}\right)^d \int_{\mathbb{R}^{3d}} \mathrm{d}p'\mathrm{d}q'\mathrm{d}p'' \exp(\frac{i}{\varepsilon}(x-z)\cdot p'')\\
&\quad \times \exp(\frac{2i}{\varepsilon}(q'-x)\cdot(p''-p'))A(q',p')\\
&\quad \times \left(\frac{\varepsilon}{2}\right)^d (2\pi)^d B(q'-\frac{1}{2}(x-z),p'')\\
&= \int_{\mathbb{R}^{3d}} \mathrm{d}p'\mathrm{d}y\mathrm{d}p'' \exp(\frac{i}{\varepsilon}(y-z)\cdot p'')\\
&\quad \times \exp(\frac{i}{\varepsilon}(x-y)\cdot p')A(\frac{1}{2}(x+y),p')B(\frac{1}{2}(y+z),p'')
\end{aligned}
$$

Here we changed the order of integration (which has to be rigorously justified in the full proof) and used the Fourier inversion formula

$$\psi(y) = (2\pi)^d \int_{\mathbb{R}^d} \mathrm{d}\lambda \int_{\mathbb{R}^d} \mathrm{d}x \exp(i\lambda\cdot(y-x))\psi(x).$$

Finally we substituted $y = 2q' - x$. On the other hand we know that

$$\begin{aligned}
&\left(\mathcal{W}^{\mathcal{S}}_{\varepsilon}(A)\mathcal{W}^{\mathcal{S}}_{\varepsilon}(B)\psi\right)(x) \\
= &\frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^{2d}} \mathrm{d}\xi\mathrm{d}y A(\frac{1}{2}(x+y),\xi)e^{\frac{i}{\varepsilon}\xi\cdot(x-y)} \\
&\times\frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^{2d}} \mathrm{d}\xi'\mathrm{d}z B(\frac{1}{2}(y+z),\xi')e^{\frac{i}{\varepsilon}\xi'\cdot(y-z)}\psi(z) \\
= &\frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^{d}} \mathrm{d}z \frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^{3d}} \mathrm{d}\xi\mathrm{d}\xi'\mathrm{d}y A(\frac{1}{2}(x+y),\xi) \\
&\times e^{\frac{i}{\varepsilon}\xi\cdot(x-y)}B(\frac{1}{2}(y+z),\xi')e^{\frac{i}{\varepsilon}\xi'\cdot(y-z)}\psi(z)
\end{aligned}$$

and a comparison gives the desired result. The norm estimate can in principle be given as the estimate in proposition (A.4). ■

Furthermore one defines the Weyl product $\widetilde{\sharp}$ between semiclassical symbols $a \in S^{w_1}(\varepsilon_0, \mathcal{L}(\mathcal{H}_3, \mathcal{H}_2))$ and $b \in S^{w_2}(\varepsilon_0, \mathcal{L}(\mathcal{H}_3, \mathcal{H}_2))$ as

$$\left(a\widetilde{\sharp}b\right)_{\varepsilon} := a_{\varepsilon}\widetilde{\sharp}_{\varepsilon}b_{\varepsilon}.$$

Note that the function $\varepsilon \mapsto \left(a\widetilde{\sharp}b\right)_{\varepsilon}$ may not be in $S^{w_1w_2}(\varepsilon_0, \mathcal{L}(\mathcal{H}_3, \mathcal{H}_1))$ although it takes values in $S^{w_1w_2}(\mathcal{L}(\mathcal{H}_3, \mathcal{H}_1))$. To following proposition shows how to expand the Weyl product in powers of ε.

Proposition A.9 *Let $A \in S^{w_1}(\mathcal{L}(\mathcal{H}_2, \mathcal{H}_3))$, $B \in S^{w_2}(\mathcal{L}(\mathcal{H}_2, \mathcal{H}_3))$. Then*

$$\sup_{\varepsilon\in(0,\varepsilon_0)} \left\| A\widetilde{\sharp}_{\varepsilon}B - \sum_{j\le n}\varepsilon^j\left(A\sharp B\right)_j \right\|_k^{(\widetilde{w})} \varepsilon^{-(n+1)} \le C_{k,n}\left\|A\right\|^{(w_1)}_{k+n+m}\left\|B\right\|^{(w_2)}_{k+n+m}$$

with m independent of n, m,

$$\widetilde{w}(q,p) = w_1(q,p)w_2(q,p)\left\langle q\right\rangle^{2(N_1+N_2)}$$

and

$$\left(A\sharp B\right)_j(q,p) := \sum_{|\alpha|+|\beta|=j}\frac{1}{\alpha!\beta!}\frac{(-1)^{|\alpha|}}{2^{|\alpha|+|\beta|}}\partial_q^{\alpha}\partial_p^{\beta}A(q,p)\partial_q^{\beta}\partial_p^{\alpha}B(q,p).$$

Proof. Once again we don't give the full proof (which can be found in [Fo], theorem 2.49) but a sketch. We start with the observation that one has, using the

Taylor expansion formula,

$$
\begin{aligned}
&A(q\prime, p\prime)B(q\prime\prime, p\prime\prime)\\
&= \sum_{|\alpha|+|\beta|\leq n} \frac{\partial_q^\alpha A(q,p')\partial_q^\beta B(q,p'')}{\alpha!\beta!}(q'-q)^\alpha(q''-q)^\beta\\
&\quad + \sum_{|\alpha|+|\beta|=n+1} |\alpha|\,|\beta| \int_0^1\int_0^1 \mathrm{d}t\mathrm{d}t' \frac{1}{\alpha!\beta!}\partial_q^\alpha A(q+t(q''-q),p')\\
&\quad \times\partial_q^\beta B(q+t'(q'-q),p'')(q'-q)^\alpha(q''-q)^\beta(1-t)^{|\alpha|-1}(1-t')^{|\beta|-1}.
\end{aligned}
$$

Inserting this result into (A.6), observing that

$$
\begin{aligned}
&(q'-q)^\alpha(q''-q)^\beta \exp(\frac{2i}{\varepsilon}(q-q\prime)^\top(p-p\prime\prime))\exp(-\frac{2i}{\varepsilon}(q-q\prime\prime)^\top(p-p\prime))\\
&= \frac{(-1)^{|\beta|}}{2^{|\alpha|+|\beta|}}\varepsilon^{|\alpha|+|\beta|}\partial_{p''}^\alpha\partial_{p'}^\beta \exp(\frac{2i}{\varepsilon}(q-q\prime)^\top(p-p\prime\prime))\exp(-\frac{2i}{\varepsilon}(q-q\prime\prime)^\top(p-p\prime))
\end{aligned}
$$

and integrating by parts we arrive at

$$
\begin{aligned}
&\left(A\widetilde{\sharp}_\varepsilon B\right)(q,p)\\
&= \left(\frac{2}{\varepsilon\pi}\right)^d \sum_{|\alpha|+|\beta|\leq n}\frac{1}{\alpha!\beta!}\frac{(-1)^{|\alpha|}}{2^{|\alpha|+|\beta|}}\varepsilon^{|\alpha|+|\beta|}\int_{\mathbb{R}^{4d}}\mathrm{d}q\prime\mathrm{d}p\prime\mathrm{d}q\prime\prime\mathrm{d}p\prime\prime\exp(\frac{2i}{\varepsilon}(q-q\prime)^\top(p-p\prime\prime))\\
&\quad\times\exp(-\frac{2i}{\varepsilon}(q-q\prime\prime)^\top(p-p\prime))\partial_q^\alpha\partial_{p'}^\beta A(q,p\prime)\partial_q^\beta\partial_{p''}^\alpha B(q,p\prime\prime)\\
&\quad+\varepsilon^{n+1}R_n(q,p)\\
&= \sum_{|\alpha|+|\beta|\leq n}\varepsilon^{|\alpha|+|\beta|}\frac{1}{\alpha!\beta!}\frac{(-1)^{|\alpha|}}{2^{|\alpha|+|\beta|}}\partial_q^\alpha\partial_p^\beta A(q,p)\partial_q^\beta\partial_p^\alpha B(q,p)\\
&\quad+\varepsilon^{n+1}R_n(q,q,p)
\end{aligned}
$$

with

$$
\begin{aligned}
&R_n(q'',q,p)\\
&= \sum_{|\alpha|+|\beta|=n+1}|\alpha|\,|\beta|\,\frac{1}{\alpha!\beta!}\frac{(-1)^{|\alpha|}}{2^{n+1}}\left(A_{\alpha,\beta}^{q''}\widetilde{\sharp}_\varepsilon B_{\beta,\alpha}^{q''}\right)(q,p)
\end{aligned}
$$

where

$$
A_{\alpha,\beta}^{q''}(q',p) = \int_0^1 \mathrm{d}t\partial_q^\alpha\partial_p^\beta A(q''+t(q'-q''),p)(1-t)^{|\alpha|-1}
$$

and $B^{q''}_{\beta,\alpha}$ defined analogously. To see that R_n is well-defined, we state that with a direct calculation

$$\left\|\partial^\gamma_{q'}\partial^\delta_p A^{q''}_{\alpha,\beta}(q',p)w_1^{-1}(q',p)\right\| \le \|A\|^{(w_1)}_{|\alpha|+|\beta|+|\gamma|+|\delta|} \langle q''\rangle^{N_1} \langle q'\rangle^{N_1},$$

i.e. $A^{q''}_{\alpha,\beta}\langle q''\rangle^{-N_1} \in S^{w_1\langle q'\rangle^{N_1}}$ uniformly in q''. The next step is to show that

$$\widetilde{R}_n(q,p) = R_n(q,q,p)$$

is differentiable and to estimate its derivatives in terms of the norms of A and B. Clearly we know that $R_n(q'',q,p)$ is smooth with respect to q and p. Furthermore, we have that

$$\begin{aligned}\partial^\gamma_{q''} A^{q''}_{\alpha,\beta}(q',p) &= \int_0^1 \mathrm{d}t \partial^{\alpha+\gamma}_q \partial^\beta_p A(q''+t(q'-q''),p)(1-t)^{|\alpha|+|\gamma|-1} \\ &= A^{q''}_{\alpha+\gamma,\beta}(q',p)\end{aligned}$$

and likewise for $B^{q''}_{\beta,\alpha}$. Furthermore, one can even show that the derivative $\partial^\gamma_{q''}A^{q''}_{\alpha,\beta}$ exists not only pointwise, but in the sense of the norms of $S^{w_1\langle q'\rangle^{N_1}}$. Together it follows that $R_n(q'',q,p)$ is smooth. This observation yields the the formula

$$\begin{aligned}&\partial^\gamma_q\partial^\delta_p\widetilde{R}_n(q,p) \\ &= \sum_{\gamma^{(1)}+\gamma^{(2)}+\gamma^{(3)}=\gamma} \frac{\gamma!}{\gamma^{(1)}!\gamma^{(2)}!\gamma^{(3)}!} \sum_{\delta'\le\delta}\binom{\delta}{\delta'} \\ &\quad\times \sum_{|\alpha|+|\beta|=n+1} |\alpha|\,|\beta| \frac{1}{\alpha!\beta!}\frac{(-1)^{|\alpha|}}{2^{n+1}} \left(\partial^{\gamma_1}_{q''}\partial^\delta_p \left(A^{q''}_{\alpha+\gamma_2,\beta}\widetilde{\sharp}_\varepsilon B^{q''}_{\beta+\gamma_3,\alpha}\right)(q,p)\right)|_{q''=q}.\end{aligned}$$

Now we can conclude with the estimate

$$\left\|\widetilde{R}_n\right\|_k^{(w_1w_2\langle q\rangle^{2(N_1+N_2)})} \le C_{k,n}\|A\|^{(w_1)}_{k+n+m}\|B\|^{(w_2)}_{k+n+m}$$

where m may depend on w_1, w_2 and d, but not on k and n. ■

For semiclassical symbols, we have the following corollary.

Corollary A.10 *Let*

$$a_\varepsilon \asymp \sum_{j=0}^\infty \varepsilon^j a_j \quad \textit{in } S^{w_1}(\varepsilon_0, \mathcal{L}(\mathcal{H}_3,\mathcal{H}_2))$$

and

$$b_\varepsilon \asymp \sum_{j=0}^{\infty} \varepsilon^j b_j \quad \text{in } S^{w_2}(\varepsilon_0, \mathcal{L}(\mathcal{H}_2, \mathcal{H}_1)),$$

then $a \widetilde{\sharp} b \in S^{\widetilde{w}}(\varepsilon_0, \mathcal{L}(\mathcal{H}_3, \mathcal{H}_1))$ *has a semiclassical expansion*

$$\left(a \widetilde{\sharp} b\right)_\varepsilon \asymp \sum_{j=0}^{\infty} \varepsilon^j \left(a \widetilde{\sharp} b\right)_k \quad \text{in } S^{\widetilde{w}}(\varepsilon_0, \mathcal{L}(\mathcal{H}_3, \mathcal{H}_1))$$

given by

$$\left(a \widetilde{\sharp} b\right)_k = \sum_{|\alpha|+|\beta|+j+l=k} \frac{1}{\alpha!\beta!} \frac{(-1)^{|\alpha|}}{2^{|\alpha|+|\beta|}} \partial_q^\alpha \partial_p^\beta A_j(q,p) \partial_q^\beta \partial_p^\alpha B_l(q,p) \tag{A.7}$$

with $k, l, j \in \mathbb{N}$ *and* $\alpha, \beta \in \mathbb{N}^d$, $\widetilde{w}(q,p) = w_1(q,p) w_2(q,p) \langle q \rangle^{2(N_1+N_2)}$.

Regarding this corollary, it makes sense to introduce the Moyal product $\sharp$: $M(\mathcal{L}(\mathcal{H}_3, \mathcal{H}_2)) \times M(\mathcal{L}(\mathcal{H}_2, \mathcal{H}_1)) \to M(\mathcal{L}(\mathcal{H}_3, \mathcal{H}_1))$ by (A.7).

B Weyl calculus for τ-equivariant symbols

In this chapter we present the special results related to τ-equivariant symbols. To this end, let $\Gamma \subset \mathbb{R}^d$ be a regular lattice, i.e.

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

Obviously, one can regard Γ as an Abelian group isomorphic to $\mathbb{Z}^d$ with addition as group operation. As in the main body of the thesis, we denote the centered fundamental cell as

$$M = \{x \in \mathbb{R}^d : x = \sum_{j=1}^{d} \alpha_j \gamma_j \text{ for } \alpha_j \in [-\frac{1}{2}, \frac{1}{2}]\}.$$

Furthermore, we assume that

$$\tau : \Gamma \to \mathcal{L}^*(\mathcal{H}_l), \quad \gamma \mapsto \tau(\gamma)$$

is a representation of the group Γ in the space of bounded invertible operators on $\mathcal{H}$, i.e. $\tau(\gamma + \gamma\prime) = \tau(\gamma)\tau(\gamma\prime)$ for all $\gamma, \gamma\prime \in \Gamma$. If more than one Hilbert space arises, then τ is a collection of such representations. Now let L_γ be the operator of translation by $\gamma \in \Gamma$ on $\mathcal{S}(\mathbb{R}^d, \mathcal{H})$, i.e. $(L_\gamma \varphi)(x) = \varphi(x - \gamma)$ resp. (without change of notation) its extension to $\mathcal{S}'(\mathbb{R}^d, \mathcal{H})$, i.e. for $T \in \mathcal{S}'(\mathbb{R}^d, \mathcal{H})$ let $(L_\gamma T)(\varphi) = T(L_{-\gamma}(\varphi))$.

Definition B.1 *A tempered distribution $T \in \mathcal{S}'(\mathbb{R}^d, \mathcal{H})$ is said to be τ-equivariant if*

$$L_\gamma T = \tau(\gamma) T \quad \text{for all } \gamma \in \Gamma,$$

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 one defines the Hilbert space

$$\mathcal{H}_\tau := \{\psi \in L^2_{loc}(\mathbb{R}^d, \mathcal{H}) : \psi(x - \gamma) = \tau(\gamma)\psi(x) \quad \text{for all } \gamma \in \Gamma\}$$

equipped with the inner product

$$\langle \varphi, \psi \rangle_{\mathcal{H}_\tau} = \int_M dx \, \langle \varphi(x), \psi(x) \rangle_{\mathcal{H}} \, .$$

Now one can easily define τ-equivariant symbols:

Definition B.2 *A symbol $A \in S^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ is τ-equivariant, if*

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

The space of τ-equivariant symbols in $S^w(\varepsilon_0, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ is denoted by

$$S^w_\tau(\varepsilon_0, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)).$$

In the same way one can of course define $S^w_\tau(\varepsilon_0, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ and $M^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ as the subspaces of $S^w_\tau(\varepsilon_0, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ resp. $M^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ where a_ε is τ-equivariant for each ε resp. A_j is τ-equivariant for each $j \in \mathbb{N}$. Note that if

$$a \asymp \sum_{j=0}^{\infty} \varepsilon^j a_j \quad \text{in } S^w(\varepsilon_0, \mathcal{L}(\mathcal{H}_2, \mathcal{H}_1))$$

and $a_\varepsilon \in S^w_\tau(\varepsilon_0, \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$, then necessarily also the coefficients a_j are in $S^w_\tau(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$ resp. $\sum_{j=0}^\infty \varepsilon^j a_j \in M^w_\tau(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$: Indeed, it follows from

$$\begin{aligned}
&\|A_0(\cdot - \gamma, \cdot) - \tau_2(\gamma) A_0 \tau_1(\gamma)\|_k^{(w)} \\
&\quad \leq \; \|A_0(\cdot - \gamma, \cdot) - a_\varepsilon(\cdot - \gamma, \cdot)\|_k^{(w)} \\
&\qquad + \|a_\varepsilon(\cdot - \gamma, \cdot) - \tau_2(\gamma) a_\varepsilon \tau_1(\gamma)\|_k^{(w)} \\
&\qquad + \|\tau_2(\gamma) a_\varepsilon \tau_1(\gamma) - \tau_2(\gamma) A_0 \tau_1(\gamma)\|_k^{(w)} \\
&\quad \leq \; C_\gamma \, \|A_0 - a_\varepsilon\|_k^{(w)} \\
&\quad \leq \; C'_\gamma \varepsilon^{-1}
\end{aligned}$$

that A_0 is τ-equivariant and inductively also for A_j, $j \geq 1$. If w depends only on q and τ is unitary we have the following result.

Lemma B.3 *Let w be an order function that is independent of p and let τ be a unitary representation. Then one has*

$$\left(\inf_{q \in M} w(q) \right) \|A\|_k^{(w)} \leq \|A\|_k^{(\mathbf{1})} \leq \left(\sup_{q \in M} w(q) \right) \|A\|_k^{(w)}, \quad k \in \mathbb{N}. \tag{B.1}$$

Proof. We have

$$\begin{aligned}\left\|\partial_q^\alpha\partial_p^\beta A(q-\gamma,p)\right\| &= \left\|\tau_2(\gamma)\partial_q^\alpha\partial_p^\beta A(q,p)\tau_1(\gamma)^{-1}\right\| \\ &= \left\|\partial_q^\alpha\partial_p^\beta A(q,p)\right\|\end{aligned}$$

for all $\gamma\in\Gamma$, therefore

$$\sup_{(q,p)\in\mathbb{R}^d}\left\|\partial_q^\alpha\partial_p^\beta A(q,p)\right\| = \sup_{q\in M,p\in\mathbb{R}^d}\left\|\partial_q^\alpha\partial_p^\beta A(q,p)\right\|$$

and the result follows. ■

Next, we want to show that the quantizations of τ-equivariant symbols preserve τ-equivariance.

Proposition B.4 *Let $A\in S^w_\tau(\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2))$, then*

$$\left(\mathcal{W}_\varepsilon^{\mathcal{S}'}(A)\right)(\mathcal{S}'_{\tau_1}(\mathbb{R}^d,\mathcal{H}_1))\subset\mathcal{S}'_{\tau_2}(\mathbb{R}^d,\mathcal{H}_2).$$

Proof. It suffices to show that $\left(L_\gamma\mathcal{W}_\varepsilon^{\mathcal{S}'}(A)T\right)(\varphi)=\left(\tau_2(\gamma)\mathcal{W}_\varepsilon^{\mathcal{S}'}(A)T\right)(\varphi)$ for all $T\in\mathcal{S}'_{\tau_1}(\mathbb{R}^d,\mathcal{H}_1)$ and $\varphi\in\mathcal{S}(\mathbb{R}^d,\mathcal{H}_2)$. We first observe that for $\mathcal{W}_\varepsilon^{\mathcal{S}}(A^*)$ and arbitrary $\psi\in\mathcal{S}(\mathbb{R}^d,\mathcal{H}_2)$

$$\begin{aligned}\left(\mathcal{W}_\varepsilon^{\mathcal{S}}(A^*)L_\gamma\psi\right)(x) &= \int_{\mathbb{R}^d}K_{A^*}(x,y)\psi(y-\gamma) \\ &= \int_{\mathbb{R}^d}K_{A^*}(x,y+\gamma)\psi(y) \\ &= \int_{\mathbb{R}^d}\left(\tau_1(\gamma)^{-1}\right)^*K_{A^*}(x-\gamma,y)\tau_2(\gamma)^*\psi(y) \\ &= \left(L_\gamma(\tau_1(\gamma)^{-1})^*\mathcal{W}_\varepsilon^{\mathcal{S}}(A^*)\tau_2(\gamma)^*\psi\right)(x).\end{aligned}$$

Here we used the fact that with

$$K_{A^*}(x,y)=\frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^d}\mathrm{d}\xi A(\frac{1}{2}(x+y),\xi)e^{\frac{i}{\varepsilon}\xi\cdot(x-y)}$$

we have

$$\begin{aligned}K_{A^*}(x-\gamma,y-\gamma) &= \frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^d}\mathrm{d}\xi A^*(\frac{1}{2}(x+y)-\gamma,\xi)e^{\frac{i}{\varepsilon}\xi\cdot(x-y)} \\ &= \left(\tau_1(\gamma)^{-1}\right)^*K_{A^*}(x,y)\tau_2(\gamma)^*.\end{aligned}$$

Now it follows by definition of $\mathcal{W}_\varepsilon^{\mathcal{S}'}(A)$ that

$$\begin{aligned}
&\left(L_\gamma \mathcal{W}_\varepsilon^{\mathcal{S}'}(A)T\right)(\varphi) \\
&= T\left(\mathcal{W}_\varepsilon^{\mathcal{S}}(A^*)L_{-\gamma}\varphi\right) \\
&= T\left(L_{-\gamma}\tau_1(\gamma)^*\mathcal{W}_\varepsilon^{\mathcal{S}}(A^*)\left(\tau_2(\gamma)^{-1}\right)^*\varphi\right) \\
&= \left(\tau_2(\gamma)\mathcal{W}_\varepsilon^{\mathcal{S}'}(A)\tau_1(\gamma)^{-1}L_\gamma T\right)(\varphi) \\
&= \left(\tau_2(\gamma)\mathcal{W}_\varepsilon^{\mathcal{S}'}(A)T\right)(\varphi).
\end{aligned}$$

■

Next we observe that the pointwise product and the Moyal product preserve τ-equivariance since translations in the phase space commute with derivatives. Similarly, also the Weyl product preserves τ-equivariance:

Proposition B.5 *Let $A \in S_\tau^{w_1}(\mathcal{L}(\mathcal{H}_3, \mathcal{H}_2))$ and $B \in S_\tau^{w_2}(\mathcal{L}(\mathcal{H}_3, \mathcal{H}_2))$, then $a\widetilde{\sharp}_\varepsilon b \in S_\tau^{w_1 w_2}(\mathcal{L}(\mathcal{H}_3, \mathcal{H}_1))$.*

Proof. We have

$$\begin{aligned}
\left(A\widetilde{\sharp}_\varepsilon B\right)(q-\gamma, p) &= \left(\frac{2}{\varepsilon\pi}\right)^d \int_{\mathbb{R}^{4d}} \mathrm{d}q\prime \mathrm{d}p\prime \mathrm{d}q\prime\prime \mathrm{d}p\prime\prime \exp(\frac{2i}{\varepsilon}(q-\gamma-q\prime)^\top(p-p\prime\prime)) \\
&\quad \times \exp(-\frac{2i}{\varepsilon}(q-\gamma-q\prime\prime)^\top(p-p\prime))A(q\prime,p\prime)B(q\prime\prime,p\prime\prime) \\
&= \left(\frac{2}{\varepsilon\pi}\right)^d \int_{\mathbb{R}^{4d}} \mathrm{d}q\prime \mathrm{d}p\prime \mathrm{d}q\prime\prime \mathrm{d}p\prime\prime \exp(\frac{2i}{\varepsilon}(q-q\prime)^\top(p-p\prime\prime)) \\
&\quad \times \exp(-\frac{2i}{\varepsilon}(q-q\prime\prime)^\top(p-p\prime))A(q\prime-\gamma,p\prime)B(q\prime\prime-\gamma,p\prime\prime) \\
&= \left(\frac{2}{\varepsilon\pi}\right)^d \int_{\mathbb{R}^{4d}} \mathrm{d}q\prime \mathrm{d}p\prime \mathrm{d}q\prime\prime \mathrm{d}p\prime\prime \exp(\frac{2i}{\varepsilon}(q-q\prime)^\top(p-p\prime\prime)) \\
&\quad \times \exp(-\frac{2i}{\varepsilon}(q-q\prime\prime)^\top(p-p\prime))\tau_3(\gamma)A(q\prime,p\prime) \\
&\quad \times \tau_2(\gamma)\tau_2(\gamma)^{-1}B(q\prime\prime,p\prime\prime)\tau_1(\gamma)^{-1} \\
&= \tau_3(\gamma)\left(A\widetilde{\sharp}_\varepsilon B\right)(q,p)\tau_1(\gamma)^{-1}.
\end{aligned}$$

■

The next important observation is that also the Calderon-Vaillancourt theorem is valid for τ-equivariant symbols.

Theorem B.6 *Let $A \in S^{\mathbf{1}}_{\tau}(\mathcal{L}(\mathcal{H}))$ and τ_1, τ_2 unitary representations of Γ in $\mathcal{L}(\mathcal{H})$, then $\mathcal{W}^{\mathcal{S}'}_{\varepsilon}(A)$ can be restricted to a bounded operator $\widehat{A}$ in $\mathcal{L}(\mathcal{H}_{\tau_1}, \mathcal{H}_{\tau_2})$ satisfying*

$$\left\|\widehat{A}\right\|_{\mathcal{L}(\mathcal{H}_{\tau_1},\mathcal{H}_{\tau_2})} \leq C_d \left\|A\right\|^{(\mathbf{1})}_{2d+1+m}$$

with C_d and m independent of A.

Proof. Let $n > \frac{d}{2}$ and $w(x) := \langle x \rangle^{-n}$. We define the Hilbert space

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

One has, for $j = 1, 2$, $\mathcal{H}_{\tau_j} \subset L^2_w$ and for any $\psi \in \mathcal{H}_{\tau_j}$ the norm equivalence

$$C_1 \left\|\psi\right\|_{\mathcal{H}_{\tau_j}} \leq \left\|\psi\right\|_{L^2_w} \leq C_2 \left\|\psi\right\|_{\mathcal{H}_{\tau_j}}$$

for appropriate finite constants C_1, C_2. The first equality is directly seen (observe that $w \neq 0$) and the second one follows from

$$\begin{aligned} \left\|\psi\right\|_{L^2_w} &= \int_{\mathbb{R}^d} \mathrm{d}x w(x)^2 \left\|\psi(x)\right\|^2_{\mathcal{H}} \\ &= \sum_{\gamma\in\Gamma} \int_{M+\gamma} \mathrm{d}x w(x)^2 \left\|\psi(x)\right\|^2_{\mathcal{H}} \\ &= \left(\sum_{\gamma\in\Gamma} \sup_{x\in M+\gamma} w(x)^2\right) \int_M \mathrm{d}x \left\|\psi(x)\right\|^2_{\mathcal{H}} \end{aligned}$$

where we used that $\left\|\psi(x)\right\|^2_{\mathcal{H}}$ is periodic because τ_j are unitary. Now it clearly suffices to estimate $\left\|\mathcal{W}^{\mathcal{S}'}_{\varepsilon}(A)\right\|_{\mathcal{L}(L^2_w)}$. Let $\psi \in C^{\infty}_{\tau_1}(\mathbb{R}^d, \mathcal{H})$, then $\mathcal{W}^{\mathcal{S}'}_{\varepsilon}(A)\psi \in C^{\infty}_{\tau_2}(\mathbb{R}^d, \mathcal{H})$ (see [Fo], theorem 2.62) and we can estimate

$$\begin{aligned} \left\|\mathcal{W}^{\mathcal{S}'}_{\varepsilon}(A)\psi\right\|_{L^2_w} &= \left\|w\mathcal{W}^{\mathcal{S}'}_{\varepsilon}(A)\psi\right\|_{L^2} \\ &\leq \left\|w\mathcal{W}^{\mathcal{S}'}_{\varepsilon}(A)w^{-1}\right\|_{\mathcal{L}(L^2)} \left\|w\psi\right\|_{L^2} \\ &= \left\|w\mathcal{W}^{\mathcal{S}'}_{\varepsilon}(A)w^{-1}\right\|_{\mathcal{L}(L^2)} \left\|\psi\right\|_{L^2_w}, \end{aligned}$$

i.e.

$$\left\|\mathcal{W}^{\mathcal{S}'}_{\varepsilon}(A)\right\|_{\mathcal{L}(L^2_w)} \leq \left\|w\mathcal{W}^{\mathcal{S}'}_{\varepsilon}(A)w^{-1}\right\|_{\mathcal{L}(L^2)}.$$

Now the usual Calderon-Vaillancourt theorem tells us that (with some $m \in \mathbb{N}$ independent of A, ε)

$$\begin{aligned} \left\| w \mathcal{W}_\varepsilon^{\mathcal{S}'}(A) w^{-1} \right\|_{\mathcal{L}(L^2)} &\leq \left\| w \widetilde{\sharp}_\varepsilon A \widetilde{\sharp}_\varepsilon w^{-1} \right\|_{2d+1}^{(\mathbf{1})} \\ &\leq \|A\|_{2d+1+m}^{(\mathbf{1})} \end{aligned}$$

where on the right hand side w is short for the symbol $(q,p) \mapsto w(q)\mathbf{1}_{\mathcal{H}}$. ■

Finally we show that for $A \in S^w_\tau(\mathcal{L}(\mathcal{H}))$ the adjoint of $\widehat{A} \in \mathcal{L}(\mathcal{H}_\tau)$, denoted by $\widehat{A}^*$ is given through the quantization of the pointwise adjoint, i.e. $\widehat{A^*}$.

Proposition B.7 *Let $A \in S^w_\tau(\mathcal{L}(\mathcal{H}))$ with a unitary representation τ and let $\widehat{A}^*$ be the adjoint of $\widehat{A} \in \mathcal{L}(\mathcal{H}_\tau)$, then $\widehat{A^*} = \widehat{A}^*$.*

Proof. Let $\psi \in \mathcal{H}_\tau$ and $\varphi \in C^\infty_\tau(\mathbb{R}^d, \mathcal{H})$ such that $\widetilde{\varphi} := \mathbf{1}_M \varphi \in C^\infty_0(\mathbb{R}^d, \mathcal{H})$, i.e. $\widetilde{\varphi}$ has support in M. For such φ we have

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

Writing the integral over $\mathbb{R}^d$ as $\int_M \mathrm{d}x \sum_{\gamma \in \Gamma}$ we have

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

Again we used that

$$K_{A^*}(x-\gamma, y-\gamma) = \left(\tau_1(\gamma)^{-1}\right)^* K_{A^*}(x,y)\tau_2(\gamma)^*$$

and the τ-equivariance of φ, ψ. Since φ with the properties from above are dense in $\mathcal{H}_\tau$ the result follows. ■

List of symbols

General notation

$\mathcal{E}$	Banach space
$\lVert\cdot\rVert_{\mathcal{E}}$	norm of the Banach space $\mathcal{E}$
$\mathcal{H}$	separable Hilbert space
$\langle\cdot,\cdot\rangle_{\mathcal{H}}$	scalar product of the Hilbert space $\mathcal{H}$
$\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)$	Banach space of bounded linear operators $A:\mathcal{H}_1\to\mathcal{H}_2$
A^*	adjoint operator in $\mathcal{L}(\mathcal{H}_2,\mathcal{H}_1)$ for $A\in\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)$
$\mathcal{D}(A)$	domain of a densely defined linear operator on $\mathcal{H}$
$\sigma(A)$	spectrum of A
$\mathrm{Tr}(A)$	trace of a trace-class operator A
$[A,B]$	commutator $[A,B]=AB-BA$ of operators A,B
$\mathbf{1}_{\mathcal{H}}$	identity operator on the Hilbert space $\mathcal{H}$
$\mathbf{1}_{\Lambda}$	characteristic function on the set Λ
$\langle\cdot\rangle$	the function $\mathbb{R}^d\to(0,\infty)$, $x\mapsto\langle x\rangle=(1+x\cdot x)^{\frac{1}{2}}$
$\mathcal{O}(\varepsilon^n)$	a function $f:(0,\varepsilon_0]\to\mathcal{E}$, $\mathcal{E}$ some normed vector space, satisfies $f(\varepsilon)=\mathcal{O}(\varepsilon^n)$ iff $\exists C<\infty$ such that $\lVert f(\varepsilon)\rVert_{\mathcal{E}}\,\varepsilon^{-n}\le C$ for all $\varepsilon\in(0,\varepsilon_0]$
$\mathcal{O}(\varepsilon^\infty)$	$f(\varepsilon)=\mathcal{O}(\varepsilon^\infty)\iff f(\varepsilon)=\mathcal{O}(\varepsilon^n)$ for all $n\in\mathbb{N}$
$\times$	Cartesian product of sets or vector product in $\mathbb{R}^3$
$\boldsymbol{\sigma}=(\boldsymbol{\sigma}_1,\boldsymbol{\sigma}_2,\boldsymbol{\sigma}_3)$	vector of Pauli spin matrices, $\boldsymbol{\sigma}_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad\boldsymbol{\sigma}_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad\boldsymbol{\sigma}_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}.$

Function spaces

O	open set in $\mathbb{R}^d$
$C^k(O,\mathcal{E})$	space of k times continuously differentiable functions $O\mapsto\mathcal{E}$
$C^k(O,\mathcal{E})$	space of k times continuously differentiable functions $O\mapsto\mathcal{E}$, that are bounded together with their derivatives
$\mathcal{S}(\mathbb{R}^d,\mathcal{H})$	Schwartz functions with values in $\mathcal{H}$
$\mathcal{S}'(\mathbb{R}^d,\mathcal{H})$	dual space of $\mathcal{S}(\mathbb{R}^d,\mathcal{H})$
$L^p(\mathbb{R}^d,\mathcal{E})$	space of functions A such that $\lVert A\rVert_{\mathcal{E}}^p$ is integrable
$H^p(\mathbb{R}^d,\mathcal{E})$	Sobolev spaces of order k

Pseudodifferential calculus

$\mathcal{W}_\varepsilon^{\mathcal{S}'}(A)$	Weyl quantization $\mathcal{W}_\varepsilon^{\mathcal{S}'}(A) : \mathcal{S}'(\mathbb{R}^d, \mathcal{H}_1) \mapsto \mathcal{S}'(\mathbb{R}^d, \mathcal{H}_2)$ of the symbol $A : \mathbb{R}^d \mapsto \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$
$\widehat{A}$ or $\mathcal{W}_\varepsilon(A)$	$\mathcal{W}_\varepsilon^{\mathcal{S}'}(A)$ restricted to an operator on $L^2(\mathbb{R}^d, \mathcal{H})$
$S^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$	space of symbols with order function w
$S(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$	$S(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)) := \bigcup_{w \text{ order function}} S^w(\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2))$
$S^w(\varepsilon_0)$	space of semiclassical symbols with order function w
$S(\varepsilon_0)$	$S(\varepsilon_0) := \bigcup_{w \text{ order function}} S^w(\varepsilon_0)$
M^w	space of formal power series with coefficients in S^w
M	$M := \bigcup_{w \text{ order function}} M^w$
$(A_\varepsilon)_n$	n-th term in the asymptotic expansion of a semiclassical symbol A_ε
$\widetilde{\sharp}$	Weyl product $\widetilde{\sharp} : S(\varepsilon) \times S(\varepsilon) \mapsto S(\varepsilon)$
$\sharp$	Moyal product $\sharp : M \times M \mapsto M$
$\{\}$	Poisson bracket

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