Effective dynamics for Bloch electrons: Peierls substitution and beyond

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December 12, 2002

Abstract

We reconsider the longstanding problem of an electron moving in a crystal under the influence of weak external electromagnetic fields. More precisely we analyze the dynamics generated by the Schrödinger operator $H = \frac{1}{2}(-\mathrm{i}\nabla_x - A(\varepsilon x))^2 + V(x) + \phi(\varepsilon x)$, where V is a lattice periodic potential and A and ϕ are external potentials which vary slowly on the scale set by the lattice spacing. We study the limit $\varepsilon \to 0$ in several steps: (i) Approximately invariant subspaces associated with isolated Bloch bands are constructed. (ii) We derive an effective quantum Hamiltonian for states inside such a decoupled subspace. The effective Hamiltonian has an asymptotic expansion in ε, starting with the term given through the Peierls substitution. Our construction allows, in principle, to compute also all higher order terms and we give the first order correction to the Peierls substitution explicitly. (iii) The semiclassical limit of the effective Hamiltonian yields the first order corrections to the "semiclassical model" of solid states physics, including a new term which has been missed in earlier heuristic studies.

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1 Introduction

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

$$\dot{q} = \nabla E_n(v)\,, \qquad \dot{v} = -\nabla\phi(q) + \dot{q}\times B(q)\,, \tag{1}$$

where $v = p - A(q)$ is the kinetic momentum and $B = \mathrm{curl A}$ is the magnetic field. (We choose units in which the Planck constant $\hbar$, the speed c of light, and the mass m of the electron are equal to one, and absorb the charge e into the potentials.) The corresponding equations of motion for the canonical variables (q,p) are generated by the Hamiltonian

$$H_{\mathrm{sc}}(q,p) = E_n\big(p - A(q)\big) + \phi(q)\,,$$

where q is the position and p the quasi-momentum of the electron. Note that there is a semiclassical evolution for each Bloch band separately.

In this article we use adiabatic perturbation theory in order to understand on a mathematical level how these semiclassical equations emerge from the underlying Schrödinger equation

$$\mathrm{i}\,\partial_s\,\psi(x,s) = \Big(\tfrac{1}{2}\big(-\mathrm{i}\nabla_x - A(\varepsilon x)\big)^2 + V_\Gamma(x) + \phi(\varepsilon x)\Big)\,\psi(x,s) \tag{2}$$

in the limit $\varepsilon \to 0$ at leading order. In addition, for the first time, the order ε correction to (1) is established, see Equation (4).

In (2) the potential $V_\Gamma : \mathbb{R}^d \to \mathbb{R}$ is periodic with respect to some regular lattice Γ generated through the basis $\{\gamma_1, \ldots, \gamma_d\}$, $\gamma_j \in \mathbb{R}^d$, i.e.

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

and $V_\Gamma(\,\cdot + \gamma) = V_\Gamma(\cdot)$ for all $\gamma \in \Gamma$. The lattice spacing defines the microscopic spatial scale. The external potentials $A(\varepsilon x)$ and $\phi(\varepsilon x)$, with $A : \mathbb{R}^d \to \mathbb{R}^d$ and $\phi : \mathbb{R}^d \to \mathbb{R}$, are slowly varying on the scale of the lattice, as expressed through the dimensionless scale parameter ε, $\varepsilon \ll 1$. In particular, this means that the external fields are weak compared to the fields generated by the ionic cores, a condition which is satisfied for real metals even for the strongest external electrostatic fields available and for a wide range of magnetic fields, cf. [AsMe], Chapter 12.

Note that the external forces due to A and ϕ are of order ε and therefore have to act over a time of order ε^{-1} to produce finite changes, which is taken as the definition of the macroscopic time scale. Hence, we will be interested in solutions of (2) for macroscopic times, but we will work mostly in the microscopic coordinates (x, s). For sake of comparison we recall that the macroscopic space-time scale (x', t) is defined through $x' = \varepsilon x$ and $t = \varepsilon s$. With this change of scale Equation (2) reads

$$\mathrm{i}\,\varepsilon\,\partial_t\,\psi^\varepsilon(x',t) = \Big(\tfrac{1}{2}\big(-\mathrm{i}\varepsilon\nabla_{x'} - A(x')\big)^2 + V_\Gamma(x'/\varepsilon) + \phi(x') \Big)\,\psi^\varepsilon(x',t) \qquad (3)$$

with initial conditions $\psi^\varepsilon(x') = \varepsilon^{-d/2}\psi(x'/\varepsilon)$. If $V_\Gamma = 0$, Equation (3) is the usual semiclassical limit with ε set equal to $\hbar$.

The problem of deriving (1) from the Schrödinger equation (2) in the limit $\varepsilon \to 0$ has been attacked along several routes. In the physics literature (1) is usually accounted for by constructing suitable semiclassical wave packets, cf. [Ko, Za]. The few mathematical approaches to the time-dependent problem (3) extend techniques from semiclassical analysis, as the WKB ansatz [GRT, DGR], or Wigner measures [GMMP], the latter being carried out only for vanishing external potentials. The large time asymptotics of the solutions to (3) without external potentials is studied in [AsKn].

In the following we will try to convince the reader that an improved understanding of the approximation must be based on the following observations. The step from (2) to (1) involves actually two limits. Semiclassical behavior can only emerge if a Bloch band is separated by a gap from the other bands and thus the corresponding subspace decouples adiabatically from its orthogonal complement. Hence we must reformulate (2) as a space-adiabatic problem. This has been done in [HST], where the semiclassical model (1) is derived for the case of zero magnetic field. The present paper is, in spirit, a continuation of the program started in [HST] to the case of both, external magnetic and electric fields. This becomes possible by reformulating the problem in such a way that the general scheme of space-adiabatic perturbation theory as developed in [PST$_1$] can be applied, granted some crucial modifications. The results we obtain in this way constitute not only the derivation of the semiclassical model in this generality, but they add, as we shall explain, new insight to the structure of the problem. In particular, we are now able to compute systematically higher order corrections in the small parameter ε to the semiclassical equations (1). The corrected equations including all terms of first order in ε read

$$\begin{aligned} \dot{q} &= \nabla_v \Big(E_n(v) - \varepsilon\, B(q) \cdot M_n(v) \Big) - \varepsilon\, \dot{v} \times \Omega_n(v)\,, \\ \dot{v} &= -\nabla_q \Big(\phi(q) - \varepsilon\, B(q) \cdot M_n(v) \Big) + \dot{q} \times B(q)\,. \end{aligned} \tag{4}$$

The Berry connection of the eigenspace-bundle corresponding to the Bloch band E_n enters in a gauge-invariant way through its curvature $\Omega_n = \mathrm{d}\mathcal{A}_n$ and through the effective magnetic moment M_n. The precise definitions of the new terms are given below in Corollary 6.

The first equation in (4) agrees with the expression found by Sundaram and Niu [SuNi], while the correction in the second equation in (4) is new. We remark that the dynamical system (1) is of interest in its own, c.f. [MaNo] and references therein, due to the nontrivial topology of the underlying phase space, and we hope that the corrections in (4) give rise to further investigations. In our paper we discuss the equations (4) only shortly at the beginning of Section 4, where we show in particular, that they are Hamiltonian with respect to a non-standard symplectic form. One concrete physical application of the refined semiclassical equations (4) is a quantitative theory for the anomalous Hall effect [JNM].

Remark 1. In the presence of a strong external magnetic field with rational flux per unit cell one formally obtains semiclassical equations identical to (4), except that the Bloch band E_n must be replaced by one of the magnetic subbands. As on striking consequence they provide the semiclassical explanation for the quantization of the Hall conductivity. More precisely, for spatial dimension $d = 2$, $\phi(q) = -\mathcal{E} \cdot q$, $B(q) = 0$, the equations of motion (4) become $\dot{q} = \nabla_v E_n(v) + \mathcal{E}^\perp \Omega_n(v)$, $\dot{v} = \mathcal{E}$, where Ω_n is now scalar and $\mathcal{E}^\perp$ is $\mathcal{E}$ rotated by $\pi/2$. We assume initially $v(0) = k$ and a completely filled band, which means to integrate with respect to k over the first Brillouin zone. Then the average current for band n is given by

$$j_n = \int \mathrm{d}k\, \dot{q}(k) = \int \mathrm{d}k\, \big(\nabla_k E_n(k) - \mathcal{E}^\perp \Omega_n(k)\big) = -\mathcal{E}^\perp \int \mathrm{d}k\, \Omega_n(k)\,.$$

$\int \mathrm{d}k\, \Omega_n(k)$ is the Chern number of the magnetic Bloch bundle and as such an integer. $\diamondsuit$

Since the precise statements of our results require considerable technical preparations, they are postponed to Section 3. At this point we only give an informal outline of the results, concluding with the theorem connecting (2) and (4).

Under Assumption (A_1) the Hamiltonian

$$H^\varepsilon = \tfrac{1}{2}\big(-\mathrm{i}\nabla_x - A(\varepsilon x)\big)^2 + V_\Gamma(x) + \phi(\varepsilon x)\,. \tag{5}$$

is self-adjoint on the domain $H^2(\mathbb{R}^d)$ and hence generates solutions to (2) in $\mathcal{H} := L^2(\mathbb{R}^d)$ through the unitary group $\mathrm{e}^{-\mathrm{i}H^\varepsilon s}$, $s \in \mathbb{R}$. As a first step we construct for each Bloch band $E_n(k)$, which does not cross or touch any other Bloch band, an orthogonal projector Π_n^ε such that the associated subspace $\Pi_n^\varepsilon\mathcal{H}$ of the full Hilbert space $\mathcal{H}$ is approximately invariant under the time evolution. More precisely, Π_n^ε satisfies

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

and thus

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

Hence transitions between $\Pi_n^\varepsilon\mathcal{H}$ and its orthogonal complement $(\Pi_n^\varepsilon\mathcal{H})^\perp$ are asymptotically smaller than any power of ε *uniformly for all initial states*. In this sense $\Pi_n^\varepsilon\mathcal{H}$ is an adiabatically decoupled subspace.

As the second step we construct an effective Hamiltonian which approximately generates the dynamics inside the band-subspace $\Pi_n^\varepsilon\mathcal{H}$. To this end we unitarily map $\Pi_n^\varepsilon\mathcal{H}$ to a suitable reference Hilbert space. In the reference representation the effective Hamiltonian is given as a pseudodifferential operator which allows for an asymptotic expansion in powers of ε. At leading order we reproduce the well known fact that the full Hamiltonian H^ε restricted to the decoupled subspace is given through the Peierls substitution, i.e.

$$H^\varepsilon \Pi_n^\varepsilon = \Big(E_n\big(-\mathrm{i}\nabla_x - A(\varepsilon x)\big) + \phi(\varepsilon x) \Big)\, \Pi_n^\varepsilon + \mathcal{O}(\varepsilon)\,, \tag{6}$$

where $\mathcal{O}(\varepsilon)$ holds in the norm of $\mathcal{B}(\mathcal{H})$, the space of bounded operators on $\mathcal{H}$. The operator $E_n\big(-\mathrm{i}\nabla_x - A(\varepsilon x)\big)$ has to be understood in the sense of Weyl quantization. However, in order to approximate the unitary time-evolution $\mathrm{e}^{-\mathrm{i}H^\varepsilon s}\Pi_n^\varepsilon$ on the decoupled subspace for finite macroscopic times $t = \varepsilon s$, the error term in (6) is not good enough and one needs in addition at least the terms of order ε. For this reason we compute explicitly the asymptotic expansion of the effective Hamiltonian up to first order terms in ε.

To state our theorem relating the Schrödinger equation (2) and the corrected semiclassical model (4) we need a few extra notations. By Γ^* we denote the dual lattice of Γ and $\Phi_n^t : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is the flow corresponding to (4). After the change of coordinates $(q, v) \mapsto (q, p) = (q, v + A(q))$ the same flow is described by

$$\overline{\Phi}_n^t(q,p) = \Big(\Phi_{n\,q}^t\big(q, p - A(q)\big),\, \Phi_{n\,v}^t\big(q, p - A(q)\big) + A(q) \Big)\,.$$

Our theorem says that the semiclassical observables are given through pseudodifferential operators with Γ^*-periodic symbols and that the Heisenberg time-evolution of such an observable is approximated by transporting the symbol along the flow (4) up to an error of order ε^2.

Theorem 2. *Let E_n be an isolated, non-degenerate Bloch band, see Definition 4, and let the potentials satisfy Assumption (A_1). Let $a \in C_\mathrm{b}^\infty(\mathbb{R}^{2d})$ be Γ^*-periodic in the second argument, i.e. $a(q, p + \gamma^*) = a(q, p)$ for all $\gamma^* \in \Gamma^*$,* *and* $\widehat{a} = a(\varepsilon x, -\mathrm{i}\nabla_x)$ *be its Weyl quantization. Then for each finite time-interval* $I \subset \mathbb{R}$ *there is a constant* $C < \infty$ *such that for* $t \in I$

$$\left\| \Pi_n^\varepsilon \left(\mathrm{e}^{\mathrm{i}H^\varepsilon t/\varepsilon}\, \widehat{a}\, \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} \,-\, \widehat{a \circ \overline{\Phi}_n^t} \right) \Pi_n^\varepsilon \right\|_{\mathcal{B}(L^2(\mathbb{R}^d))} \leq \varepsilon^2\, C\,.$$

In particular, for $\psi_0 \in \Pi_n^\varepsilon \mathcal{H}$ *we have that*

$$\left| \left\langle \psi_0,\, \mathrm{e}^{\mathrm{i}H^\varepsilon t/\varepsilon}\, \widehat{a}\, \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon}\, \psi_0 \right\rangle - \left\langle \psi_0,\, \widehat{a \circ \overline{\Phi}_n^t}\, \psi_0 \right\rangle \right| \leq \varepsilon^2\, C\, \|\psi_0\|^2\,.$$

To our knowledge, Theorem 2 is the first rigorous result relating the full time-dependent Schrödinger equation (2) to the semiclassical model (1) for general external magnetic and electric fields and the first result to include the first order correction.

We remark that the time-*independent* problem was solved in [GMS], with predecessors [BeRa, Bu, HeSj, Ne]. In this case the goal is to obtain an effective Hamiltonian with the same spectrum as H^ε closed to some prescribed energy.

We end the introduction with a brief outline of the paper. In Section 2 we discuss the periodic Hamiltonian, i.e. (5) without A and ϕ. In particular we recall the unitary Bloch-Floquet transformation and explain our assumptions in detail. In Section 3 we apply the general scheme of space-adiabatic perturbation theory as developed in [PST_1] to the present setting. This contains the construction of the decoupled subspace and of the effective Hamiltonian generating the intraband dynamics to all orders in ε. The key observation for applying space-adiabatic perturbation theory is that the Hamiltonian H^ε can be written, after a suitable Bloch-Floquet transformation, as the Weyl quantization of an operator-valued symbol. However, the underlying Hilbert space is not of the form $L^2(\mathbb{R}^d, \mathcal{H}_\mathrm{f})$, as for standard pseudodifferential operators, but $L^2(B, \mathcal{H}_\mathrm{f})$, where B is the first Brillouin zone, the fundamental domain of the dual lattice Γ^*. Our symbols are not functions on the phase space $\mathbb{R}^d \times \mathbb{R}^d$, but, roughly speaking, on $B \times \mathbb{R}^d$. Hence a suitable version of the parameter dependent pseudodifferential calculus is developed in the Appendix. Finally, in Section 4 we discuss the semiclassical limit of the effective intraband Hamiltonian and prove, in particular, Theorem 2.

2 The periodic Bloch Hamiltonian

In order to formulate our assumptions and our results we first need to recall several well known facts about the periodic Hamiltonian

$$H_\mathrm{per} := -\frac{1}{2}\Delta + V_\Gamma\,,$$

i.e. about (5) without the non-periodic perturbations A and ϕ.

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

$$M = \Big\{ x \in \mathbb{R}^d : x = \textstyle\sum_{j=1}^d \alpha_j \, \gamma_j \ \text{ for } \alpha_j \in [-\frac{1}{2}, \frac{1}{2}] \Big\} ,$$

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

The Bloch-Floquet transform of a function $\psi \in \mathcal{S}(\mathbb{R}^d)$ is defined as

$$(\mathcal{U}\psi)(k, x) := \sum_{\gamma \in \Gamma} \mathrm{e}^{-\mathrm{i}(x+\gamma)\cdot k} \psi(x + \gamma), \ \ (k, x) \in \mathbb{R}^{2d} \tag{7}$$

and one directly reads off from (7) the following periodicity properties:

$$\big(\mathcal{U}\psi\big)(k, y + \gamma) = \big(\mathcal{U}\psi\big)(k, y) \qquad \text{for all} \quad \gamma \in \Gamma \, , \tag{8}$$

$$\big(\mathcal{U}\psi\big)(k + \gamma^*, y) = \mathrm{e}^{-\mathrm{i}y\cdot\gamma^*} \, \big(\mathcal{U}\psi\big)(k, y) \qquad \text{for all} \quad \gamma^* \in \Gamma^* \, . \tag{9}$$

From (8) it follows that, for any fixed $k \in \mathbb{R}^d$, $\big(\mathcal{U}\psi\big)(k, \cdot)$, is a Γ-periodic function and can then be regarded as an element of $L^2(\mathbb{T}^d)$, $\mathbb{T}^d$ being the flat torus $\mathbb{R}^d/\Gamma$.

Equation (9) involves a unitary representation of the group of lattice translation on Γ^* (denoted again as Γ^* with a little abuse of notation), given by

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

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

$$\mathcal{H}_\tau := \Big\{ \psi \in L^2_{\mathrm{loc}}(\mathbb{R}^d, L^2(\mathbb{T}^d)) : \ \psi(k - \gamma^*) = \tau(\gamma^*) \, \psi(k) \Big\} \, , \tag{10}$$

equipped with the inner product

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

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

Obviously, there is a natural isomorphism between $\mathcal{H}_\tau$ and $L^2(B, L^2(\mathbb{T}^d))$ given by restriction from $\mathbb{R}^d$ to B, and with inverse given by τ-equivariant continuation, as suggested by (9). The reason for working with $\mathcal{H}_\tau$ instead of $L^2(B, L^2(\mathbb{T}^d))$ is twofold. First of all it allows to apply the pseudodifferential calculus as developed in the Appendix. On the other hand it makes statements about domains of operators more transparent as we shall see.

The map defined by (7) extends to a unitary operator

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

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

$$\big(\mathcal{U}^{-1}\varphi\big)(x) = \int_B \mathrm{d}k\ \mathrm{e}^{\mathrm{i}x\cdot k}\,\varphi(k,[x]) \tag{11}$$

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

In order to determine the Bloch-Floquet transform for operators like the full Hamiltonian (5), we need to discuss how differential and multiplication operators behave under Bloch-Floquet transformation. The following assertions follow in a straightforward way from the definition (7). Let $P = -\mathrm{i}\nabla_x$ with domain $H^1(\mathbb{R}^d)$ and Q be multiplication with x on the maximal domain, then

$$\begin{aligned} \mathcal{U}\,P\,\mathcal{U}^{-1} &= \mathbf{1} \otimes -\mathrm{i}\nabla_y^{\mathrm{per}} + k \otimes \mathbf{1}\,, && (12)\\ \mathcal{U}\,Q\,\mathcal{U}^{-1} &= \mathrm{i}\nabla_k^{\tau}\,, && (13) \end{aligned}$$

where $-\mathrm{i}\nabla_y^{\mathrm{per}}$ is equipped with periodic boundary conditions or, equivalently, operating on the domain $H^1(\mathbb{T}^d)$. The domain of $\mathrm{i}\nabla_k^\tau$ is $\mathcal{H}_\tau \cap H^1_{\mathrm{loc}}(\mathbb{R}^d, L^2(\mathbb{T}))$, i.e. it consists of distributions in $H^1(B, L^2(\mathbb{T}^d))$ which satisfy the y-dependent boundary condition associated with (9).

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

For later use we remark that the following relations can be checked using the definitions (7) and (11):

$$\begin{aligned} \psi \in H^m(\mathbb{R}^d)\,,\ m \geq 0 \quad &\Longleftrightarrow \quad \mathcal{U}\psi \in L^2(B, H^m(\mathbb{T}))\,,\\ \langle x\rangle^m \psi(x) \in L^2(\mathbb{R}^d)\,,\ m \geq 0 \quad &\Longleftrightarrow \quad \mathcal{U}\psi \in \mathcal{H}_\tau \cap H^m_{\mathrm{loc}}(\mathbb{R}^d, L^2(\mathbb{T}))\,. \end{aligned}$$

Remark 3. Often the Bloch-Floquet transformation is defined for $\psi \in \mathcal{S}(\mathbb{R}^d)$ as

$$(\widetilde{\mathcal{U}}\psi)(k,x) := \sum_{\gamma\in\Gamma} \mathrm{e}^{-\mathrm{i}x\cdot k}\psi(x+\gamma),\ \ (k,x) \in \mathbb{R}^{2d}\,. \tag{14}$$

In contrast to (7), functions in the range of $\widetilde{\mathcal{U}}$ are periodic in k and quasi-periodic in y:

$$\begin{aligned} \big(\widetilde{\mathcal{U}}\psi\big)(k, y+\gamma) = \mathrm{e}^{\mathrm{i}k\cdot\gamma}\,\big(\widetilde{\mathcal{U}}\psi\big)(k,y) \quad &\text{for all} \quad \gamma \in \Gamma\,, && (15)\\ \big(\widetilde{\mathcal{U}}\psi\big)(k+\gamma^*, y) = \big(\widetilde{\mathcal{U}}\psi\big)(k,y) \quad &\text{for all} \quad \gamma^* \in \Gamma^*\,. && (16) \end{aligned}$$

Our choice of $\mathcal{U}$ instead of $\widetilde{\mathcal{U}}$ comes from the fact, that the transform of the gradient has a domain which is independent of $k \in B$, cf. (12). This is, as we shall see, essential for an application of the pseudodifferential calculus of the Appendix. $\diamondsuit$

For the Bloch-Floquet transform of the free Hamiltonian one finds

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

with

$$H_{\mathrm{per}}(k) = \frac{1}{2}\big(- \mathrm{i}\nabla_y + k\big)^2 + V_\Gamma(y)\,, \quad k \in B\,. \tag{17}$$

For fixed $k \in B$ the operator $H_{\mathrm{per}}(k)$ acts on $L^2(\mathbb{T}^d)$ with domain $H^2(\mathbb{T}^d)$ independent of $k \in B$, whenever the following assumption on the potential is satisfied.

Assumption ($\mathbf{A}_1$). *We assume that V_Γ is infinitesimally bounded with respect to $-\Delta$ and that $\phi \in C^\infty_{\mathrm{b}}(\mathbb{R}^d, \mathbb{R})$ and $A_j \in C^\infty_{\mathrm{b}}(\mathbb{R}^d, \mathbb{R})$ for any $j \in \{1, \ldots, d\}$.*

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

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

$$H_{\mathrm{per}}(k - \gamma^*) = \tau(\gamma^*)\, H_{\mathrm{per}}(k)\, \tau(\gamma^*)^{-1}\,, \tag{18}$$

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

Definition 4. We say that a band $E_n(k)$ or a group of bands $\{E_n(k)\}_{n\in\mathcal{I}}$, $\mathcal{I} = [I_-, I_+] \cap \mathbb{N}$, is an **isolated Bloch band** or **satisfies the gap condition**, if

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

For the following we fix an index set $\mathcal{I} \subset \mathbb{N}$ corresponding to an isolated group of bands. Let $P_\mathcal{I}(k)$ be the spectral projector of $H_{\mathrm{per}}(k)$ corresponding to the eigenvalues $\{E_n(k)\}_{n\in\mathcal{I}}$, then $P_\mathcal{I} := \int_B^\oplus \mathrm{d}k\, P_\mathcal{I}(k)$ is the projector on the given isolated Bloch band.

In terms of Bloch functions, one has that $P_\mathcal{I}(k) = \sum_{n\in\mathcal{I}} |\varphi_n(k)\rangle\langle\varphi_n(k)|$. However, in general, $\varphi_n(k)$ are not smooth functions of k at eigenvalue crossings, while $P_{\mathcal{I}}(k)$ is a smooth function of k because of the gap condition. Moreover, from (18) it follows that

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

For the mapping to the reference space we will need the following assumption.

Assumption (A_2). *If $d>1$ and if the isolated group of Bloch bands $\{E_n(k)\}_{n\in\mathcal{I}}$ is degenerate in the sense that $\ell := |\mathcal{I}| > 1$, then we assume that there exists an orthonormal basis $\{\psi_j(k)\}_{j=1}^{\ell}$ of $\mathrm{Ran}P_{\mathcal{I}}(k)$ whose elements are smooth and τ-equivariant with respect to k, i.e. $\psi_j(k-\gamma^*) = \tau(\gamma^*)\psi_j(k)$ for all $j\in\{1,\dots,\ell\}$ and $\gamma^*\in\Gamma^*$.*

In the special but important case in which the relevant band consist of an isolated ℓ-fold degenerate eigenvalue (i.e. $E_n(k) = E_*(k)$ for every $n\in\mathcal{I}$, $|\mathcal{I}|=\ell$), Assumption (A_2) is equivalent to the existence of an orthonormal basis consisting of smooth and τ-equivariant Bloch functions. In the general case, in which *eigenvalue crossings* inside the relevant band are present, Assumption (A_2) is weaker, since it is not required that $\psi_j(k)$ is an eigenfunction of the free Hamiltonian $H_{\mathrm{per}}(k)$, but only of the corresponding eigenprojection $P_{\mathcal{I}}(k)$.

We expect that Assumption (A_2) is generically satisfied, i.e. the eigenvector bundles corresponding to isolated Bloch bands are trivial. For $d=1$ this follows from the fact that all $U(n)$-bundles with base space S^1 are trivial. For $\ell=1$ the bundle must be trivial, since the first Chern class vanishes as a consequence of time-reversal invariance. The latter statements are a geometric reformulation of a, infact slightly stronger, result by Nenciu [Ne]. A more detailed study of the geometry of Bloch bundles exceeds the scope of this paper and is postponed to a forthcoming paper.

In the presence of a strong external magnetic field the Bloch bands split into magnetic sub-bands. Generically, their first Chern number does not vanish and therefore Assumption (A_2) fails. As well understood, the nonvanishing of the first Chern number is directly linked to the integer quantum Hall effect [TKNN, Si], hence our interest in extending Theorem 3 to magnetic Bloch bands. The required modifications of our theory will be discussed in [PST_3].

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

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

Notice, however, that P_n is not a spectral subspace of H_{per}, in general.

According to Proposition 14, in the original representation H_{per} acts on the n^{th} band subspace as

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

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

3 Space-adiabatic perturbation for Bloch bands

In the presence of non-periodic external fields the subspaces $P_n\mathcal{H}$ are no longer invariant, since the external fields induce transitions between different band subspaces. If the potentials are varying slowly, these transitions are small and one expects that there still exist approximately invariant subspaces associated with isolated Bloch bands. The dynamics of states inside the decoupled subspaces should be generated by an effective Hamiltonian given through the Peierls substitution as in (6).

In this section we apply the general scheme of adiabatic perturbation theory as developed in [PST$_1$] to the problem of perturbed Bloch bands in order to rigorously justify the heuristic picture.

We first present a theorem which summarizes the main results of this section. The remaining parts give the results and the proofs of the three main steps in space-adiabatic perturbation theory: In Section 3.1 we construct the almost invariant subspaces associated with isolated Bloch bands. In Section 3.2 we explain how to unitarily map the decoupled subspace to a suitable reference Hilbert space. In this reference representation the action of the full Hamiltonian is given through a semiclassical pseudodifferential operator, whose expansion can be computed to any order in ε. This effective Hamiltonian is constructed in Section 3.3 and we compute its asymptotic expansion explicitly including the subprincipal symbol. For a detailed presentation of the general idea we refer to [PST$_1$] and [Te]. The main technical innovation necessary in order to apply the scheme to the present case is the development of a pseudodifferential calculus for operators acting on sections of a bundle over the flat torus B, or, equivalently, acting on the space $\mathcal{H}_\tau$. This is done in the Appendix.

Before going into the details of the construction we present a theorem which encompasses the main results of this section. Generalizing from (10) it is convenient to introduce the following notation. For any separable Hilbert space $\mathcal{H}_\mathrm{f}$ and any unitary representation $\tau : \Gamma^* \to \mathcal{U}(\mathcal{H}_\mathrm{f})$, one defines the Hilbert space

$$L^2_\tau(\mathbb{R}^d, \mathcal{H}_\mathrm{f}) := \Big\{ \psi \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathcal{H}_\mathrm{f}) : \ \psi(k - \gamma^*) = \tau(\gamma^*)\, \psi(k) \Big\} ,$$

equipped with the inner product

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

Using the results of the previous section and imposing Assumption (A$_1$), the Bloch-Floquet transform of the full Hamiltonian (5) is given through

$$H^\varepsilon_{\mathrm{BF}} := \mathcal{U}\, H^\varepsilon\, \mathcal{U}^{-1} = \frac{1}{2}\Big(-\mathrm{i}\nabla_y + k - A\big(\mathrm{i}\varepsilon\nabla^\tau_k\big)\Big)^2 + V_\Gamma(y) + \phi\big(\mathrm{i}\varepsilon\nabla^\tau_k\big) \qquad (19)$$

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

The application of space-adiabatic perturbation theory to an isolated group of bands $\{E_n(k)\}_{n\in\mathcal{I}}$ yields the following result, where the reference Hilbert space for the effective dynamics is $\mathcal{K} := L^2(\mathbb{T}^d) \otimes \mathbb{C}^\ell$ with $\ell := \dim P_\mathcal{I}(k)$.

Theorem 5 (Peierls substitution and higher order corrections). *Let $\{E_n\}_{n\in\mathcal{I}}$ be an isolated group of bands, see Definition 4, and let Assumptions (A_1) and (A_2) be satisfied. Then there exist*

(i) *an orthogonal projection $\Pi \in \mathcal{B}(\mathcal{H}_\tau)$,*

(ii) *a unitary map $U \in \mathcal{B}(\Pi\mathcal{H}_\tau, \mathcal{K})$, and*

(iii) *a self-adjoint operator $\widehat{h} \in \mathcal{B}(\mathcal{K})$*

such that

$$\big\| \big[H^\varepsilon_{\mathrm{BF}}, \Pi \big] \big\| = \mathcal{O}(\varepsilon^\infty)\,, \qquad \| \Pi - P_{\mathcal{I}} \| = \mathcal{O}(\varepsilon)$$

and

$$\big\| \big(e^{-iH^\varepsilon_{\mathrm{BF}} t} - U^* \; e^{-i\widehat{h}t} \; U \big) \Pi \big\| = \mathcal{O}(\varepsilon^\infty (1 + |t|)).$$

The effective Hamiltonian $\widehat{h}$ is the Weyl quantization of a semiclassical symbol $h \in S^1_{\tau\equiv\mathbf{1}}(\varepsilon, \mathcal{B}(\mathbb{C}^\ell))$ with an asymptotic expansion which can be computed to any order. The $\mathcal{B}(\mathbb{C}^\ell)$-valued principal symbol $h_0(k,r)$ has matrix-elements

$$h_0(k,r)_{\alpha\beta} = \big\langle \psi_\alpha(k - A(r)), H_0(k,r)\, \psi_\beta(k - A(r)) \big\rangle\,, \tag{20}$$

where $\alpha, \beta \in \{1, \ldots, \ell\}$ and $H_0(k,r)$ is defined in (24).

The general formula for the subprincipal symbol of the effective Hamiltonian can be found in [PST$_1$]. The structure and the interpretation of the effective Hamiltonian are most transparent for the case of a single isolated band.

Corollary 6. *For an isolated ℓ-fold degenerate eigenvalue $E(k)$ the $\mathcal{B}(\mathbb{C}^\ell)$-valued symbol $h(k,r) = h_0(k,r) + \varepsilon h_1(k,r) + \mathcal{O}_0(\varepsilon^2)$ constructed in Theorem 5 has matrix-elements*

$$h_0(k,r)_{\alpha\beta} = \big(E(k - A(r)) + \phi(r) \big) \delta_{\alpha\beta} \tag{21}$$

and

$$h_1(k,r)_{\alpha\beta} = \big(\nabla\phi(r) - \nabla E(\widetilde{k}) \times B(r) \big) \cdot \mathcal{A}(\widetilde{k})_{\alpha\beta} - B(r) \cdot M(\widetilde{k})_{\alpha\beta} \tag{22}$$

$$\begin{aligned} := \quad & \Big(\partial_j \phi(r) - \partial_l E(\widetilde{k}) \, \big(\partial_j A_l(r) - \partial_l A_j(r) \big) \Big) \, \mathcal{A}_j(\widetilde{k})_{\alpha\beta} \\ & - \big(\partial_j A_l - \partial_l A_j \big)(r) \; \mathrm{Re} \Big[\tfrac{\mathrm{i}}{2} \, \big\langle \partial_l \psi_\alpha(\widetilde{k}), (H_{\mathrm{per}} - E)(\widetilde{k}) \; \partial_j \psi_\beta(\widetilde{k}) \big\rangle_{\mathcal{H}_{\mathrm{f}}} \Big]\,, \end{aligned}$$

where summation over indices appearing twice is implicit, $\widetilde{k} = k - A(r)$, and $\alpha, \beta \in \{1, \ldots, \ell\}$. The coefficients of the Berry connection are

$$\mathcal{A}(k)_{\alpha\beta} = \mathrm{i} \, \big\langle \psi_\alpha(k), \nabla \psi_\beta(k) \big\rangle_{\mathcal{H}_{\mathrm{f}}}\,. \tag{23}$$

In dimension $d = 3$ the subprincipal symbol (22) has a straight forward physical interpretation. The 2-forms B and M are naturally identified with the vectors $B = \mathrm{curl} A$ and

$$M(k)_{\alpha\beta} = \tfrac{\mathrm{i}}{2} \left\langle \nabla\psi_\alpha(k),\ \times (H_{\mathrm{per}}(k) - E(k)) \nabla\psi_\beta(k) \right\rangle_{\mathcal{H}_{\mathrm{f}}} .$$

Then the symbol of the effective Hamiltonian has a form reminiscent of the one obtained from a multipole expansion for a classical charge distribution in weak external fields. In this sense one can interpret $\mathcal{A}(k)$ as an effective electric dipole moment and $M(k)$ as an effective magnetic dipole moment. We do not know if this analogy carries on to the higher order terms.

Remark 7. Our results hold for arbitrary dimension d. However, to simplify presentation, we use a notation motivated by the vector product and the duality between 1-forms and 2-forms for $d = 3$. If $d \neq 3$, then B, Ω_n and M_n are 2-forms. The inner product of 2-forms is

$$B \cdot M := *^{-1}(B \wedge *M) = \sum_{j=1}^{d} \sum_{i=1}^{d} B_{ij} M_{ij} \,,$$

where $*$ denotes the Hodge duality induced by the euclidian metric, and for a vector field w and a 2-form F the "vector product" is

$$(w \times F)_j := (*^{-1}(w \wedge *F))_j = \sum_{i=1}^{d} w_i F_{ij} \,,$$

where the duality between 1-forms and vector fields was used implicitly. $\diamondsuit$

We remark that E. I. Blount [Bl_1, Bl_2] derived the same effective Hamiltonian for isolated Bloch bands through a formal diagonalization of the full Hamiltonian in the Bloch-Floquet representation. It seems that his work remained largely unnoticed due to its complexity.

Theorem 5 is a direct consequence of the results proved in Propositions 8, 10 and 11. The proof of Corollary 6 is given at the end of this section.

As explained before, the main idea of the proof is to adapt the general scheme of space-adiabatic perturbation theory of [PST_1] to the case of the Bloch electron. While formally this seems straightforward, one must overcome two mathematical problems. First of all, in the present case the symbols are *unbounded*-operator-valued functions. One can deal with unbounded-operator-valued symbols by considering them as bounded operators from their domain equipped with the graph norm into the Hilbert space, cf. e.g. [DiSj].

The second, more serious problem consists in setting up a Weyl calculus for operators acting on spaces like $L^2_\tau(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}})$. This is done in the Appendix and we will use in this section terminology and notations introduced there.

The results of the Appendix allow us to write the Hamiltonian $H^\varepsilon_{\mathrm{BF}}$ as the Weyl quantization $H_0(k, \mathrm{i}\varepsilon\nabla_k)$ of the τ-equivariant symbol

$$H_0(k, r) = \frac{1}{2} \left(-\mathrm{i}\nabla_x + k - A(r)\right)^2 + V_\Gamma(x) + \phi(r) \tag{24}$$

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

$$\widehat{H}_0 = \frac{1}{2}\Big(-\mathrm{i}\nabla_y + k - A\big(\mathrm{i}\varepsilon\nabla_k\big)\Big)^2 + V_\Gamma(y) + \phi\big(\mathrm{i}\varepsilon\nabla_k\big)\,. \tag{25}$$

Then $\widehat{H}_0$ can be restricted to $L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathcal{D})$, since A and ϕ are smooth and bounded. Since H_0 is a τ-equivariant symbol, $\widehat{H}_0$ preserves τ-equivariance and can then be restricted to an operator from $L^2_\tau(\mathbb{R}^d, \mathcal{D})$ to $L^2_\tau(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}})$. To conclude that (25), restricted to $L^2_\tau(\mathbb{R}^d, \mathcal{D})$, agrees with (19), it is enough to recall that $\mathrm{i}\nabla^\tau_k$ is defined as $\mathrm{i}\nabla_k$ restricted to $H^1 \cap \mathcal{H}_\tau$ and to use the spectral calculus.

Moreover, if one introduces the order function $w(k, r) := (1 + k^2)$, then $H_0 \in S^w_\tau(\mathcal{B}(\mathcal{D}, \mathcal{H}))$. More generally, we will give the proofs for any symbol $H \in S^w_\tau(\varepsilon, \mathcal{B}(\mathcal{D}, \mathcal{H}))$, whose principal symbol is then denoted by H_0.

We now proceed along the lines of the general scheme of [PST$_1$]. The basic strategy of the proof remains unchanged, but several important technical details are different.

3.1 The almost invariant subspace

In this section we construct the adiabatically decoupled subspace associated with an isolated group of bands. Similar constructions have a considerable history and we refer to [MaSo, NeSo, PST$_1$] for references.

Given an isolated group of bands $\{E_n(k)\}_{n\in\mathcal{I}}$, we change notation and define $\pi_0(k, r) = P_{\mathcal{I}}(k - A(r))$. It follows from the τ-equivariance of H_0 and from the gap condition that $\pi_0 \in S^1_\tau(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$. We also define the shorthand $A(\varepsilon) = \mathcal{O}_0(\varepsilon^n)$, where the subscript 0 expresses that a family $A(\varepsilon) \subset \mathcal{B}(\mathcal{H})$ is $\mathcal{O}(\varepsilon^n)$ in the norm of bounded operators.

Proposition 8. *Let $\{E_n\}_{n\in\mathcal{I}}$ be an isolated group of bands and let Assumption (A_1) be satisfied. Then there exists an orthogonal projection $\Pi \in \mathcal{B}(\mathcal{H}_\tau)$ such that*

$$\big[\, H^\varepsilon_{\mathrm{BF}}, \Pi \,\big] = \mathcal{O}_0(\varepsilon^\infty) \tag{26}$$

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

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

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

Proof. We first construct π on a formal symbol level.

Lemma 9. *Let $w(k,r) = (1+k^2)$. There exists a* unique *formal symbol*

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

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

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

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

(iii) $H \,\sharp\, \pi - \pi \,\sharp\, H = 0$.

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

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

$$\mathrm{dist}\big(\Lambda(z_0), \sigma(H(z))\big) \geq \frac{1}{4} C_\mathrm{g} \quad \text{for all} \quad z \in \mathcal{U}_{z_0} \tag{27}$$

and

$$\mathrm{Radius}(\Lambda(z_0)) \leq C_\mathrm{r}\,. \tag{28}$$

The constant C_g appearing in (27) is the same as in Definition 4 and the existence of a constant C_r independent of z_0 such that (28) is satisfied follows from the periodicity of $\{E_n(z)\}_{n\in\mathcal{I}}$ and the fact that A and ϕ are bounded. Indeed, Λ can be chosen Γ^*-periodic, i.e. such that $\Lambda(k_0 + \gamma^*, r_0) = \Lambda(k_0, r_0)$ for all $\gamma^* \in \Gamma^*$.

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

$$(H - \zeta) \,\sharp\, R(\zeta) = \mathbf{1}_{\mathcal{H}_\mathrm{f}} \quad \text{and} \quad R(\zeta) \,\sharp\, (H - \zeta) = \mathbf{1}_\mathcal{D} \quad \text{on } \mathcal{U}_{z_0}\,. \tag{29}$$

To this end let

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

where according to (27) $R_0(\zeta)(z) \in \mathcal{B}(\mathcal{H}_\mathrm{f}, \mathcal{D})$ for all $z \in \mathcal{U}_{z_0}$, and, using differentiability of $H(z)$, $\partial_z^\alpha R_0(\zeta)(z) \in \mathcal{B}(\mathcal{H}_\mathrm{f}, \mathcal{D})$ for all $z \in \mathcal{U}_{z_0}$. By construction one has

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

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

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

with $R_j(\zeta)(z) \in \mathcal{B}(\mathcal{H}_\mathrm{f}, \mathcal{D})$ for all $z \in \mathcal{U}_{z_0}$ satisfies the first equality in (29) up to $\mathcal{O}(\varepsilon^{n+1})$, i.e.

$$(H - \zeta) \sharp R^{(n)}(\zeta) = \mathbf{1}_{\mathcal{H}_\mathrm{f}} + \varepsilon^{n+1} E_{n+1}(\zeta) + \mathcal{O}_0(\varepsilon^{n+2}) \,, \tag{30}$$

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

$$R_{n+1}(\zeta) = -R_0(\zeta)\, E_{n+1} \tag{31}$$

we obtain that $R^{(n+1)}(\zeta) = R^{(n)}(\zeta) + \varepsilon^{n+1} R_{n+1}(\zeta)$ takes values in $\mathcal{B}(\mathcal{H}_\mathrm{f}, \mathcal{D})$ and satisfies the first equality in (29) up to $\mathcal{O}(\varepsilon^{n+2})$. Hence the formal symbol $R(\zeta) = \sum_{j=0}^{\infty} \varepsilon^j R_j(\zeta)$ constructed that way satisfies the first equality in (29) exactly. By the same argument one shows that there exists a formal symbol $\widetilde{R}(\zeta)$ with values in $\mathcal{B}(\mathcal{H}_\mathrm{f}, \mathcal{D})$ which exactly satisfies the second equality in (29). By the associativity of the Moyal product, they must agree:

$$\widetilde{R}(\zeta) = \widetilde{R}(\zeta) \sharp (H - \zeta) \sharp R(\zeta) = R(\zeta) \qquad \text{on } \mathcal{U}_{z_0}.$$

Equations (29) imply that $R(\zeta)$ satisfies the resolvent equation

$$R(\zeta) - R(\zeta') = (\zeta - \zeta')\, R(\zeta) \sharp R(\zeta') \quad \text{on } \mathcal{U}_{z_0} \tag{32}$$

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

$$\pi_j(z) := \frac{\mathrm{i}}{2\pi} \oint_{\Lambda(z_0)} \mathrm{d}\zeta\, R_j(\zeta, z) \quad \text{on } \mathcal{U}_{z_0} \tag{33}$$

satisfies (i) and (ii) of Lemma 9. As for (iii) a little bit of care is required. Let $J : \mathcal{D} \to \mathcal{H}_\mathrm{f}$ be the continuous injection of $\mathcal{D}$ into $\mathcal{H}_\mathrm{f}$. Using (33) and (32) it follows that $\pi\, J \sharp R(\zeta) = R(\zeta)\, J \sharp \pi$ for all $\zeta \in \Lambda(z_0)$. Moyal-multiplying from left and from the right with $H - \zeta$ one finds $H \sharp \pi\, J = J\, \pi \sharp H$ as operators in $\mathcal{B}(\mathcal{D}, \mathcal{H}_\mathrm{f})$. However, by construction $H \sharp \pi$ takes values in $\mathcal{B}(\mathcal{H}_\mathrm{f})$ and, by density of $\mathcal{D}$, the same must be true for $\pi \sharp H$.

We are left to show that $\pi \in M^1_\tau(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f})) \cap M^w_\tau(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}, \mathcal{D}))$. To this end notice that by construction π inherits the τ-equivariance of H, i.e.

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

From (33) and (28) we conclude that for each $\alpha \in \mathbb{N}^{2d}$ and $j \in \mathbb{N}$ one has

$$\|(\partial_z^\alpha \pi_j)(z)\| \le 2\pi C_\mathrm{r} \sup_{\zeta \in \Lambda(z_0)} \|(\partial_z^\alpha R_j)(\zeta, z)\| \,, \tag{34}$$

where $\|\cdot\|$ stands either for the norm of $\mathcal{B}(\mathcal{H}_\mathrm{f})$ or for the norm of $\mathcal{B}(\mathcal{H}_\mathrm{f}, \mathcal{D})$. In order to show that $\pi \in M^1_\tau(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}))$ it suffices to consider $z = (k, r) \in B \times \mathbb{R}^d$ since $\tau(\gamma^*)$ is unitary and thus the $\mathcal{B}(\mathcal{H}_\mathrm{f})$-norm of π is periodic. According to (34) we must show that

$$\|(\partial_z^\alpha R_j)(\zeta, z)\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} \le C_{\alpha j} \quad \forall\, z \in \mathcal{U}_{z_0},\, \zeta \in \Lambda(z_0) \tag{35}$$

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

We prove (35) by induction. Assume, by induction hypothesis, that for any $j \leq n$ one has that

$$R_j(\zeta) \in S^1_\tau(\mathcal{B}(\mathcal{H}_\mathrm{f})) \cap S^w_\tau(\mathcal{B}(\mathcal{H}_\mathrm{f}, \mathcal{D})) \tag{36}$$

uniformly in ζ, in the sense that the Fréchet semi-norms are bounded by ζ-independent constants. Then, according to Proposition 25, $E_{n+1}(\zeta)$, as defined by (30), belongs to $S^{w^2}_\tau(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ uniformly in ζ. By τ-equivariance, the norm of $E_{n+1}(\zeta)$ is periodic and one concludes that $E_{n+1}(\zeta) \in S^1_\tau(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ uniformly in ζ. It follows from (31) that (36) is satisfied for $j = n+1$.

We are left to show that (36) is fulfilled for $j = 0$. We notice that according to (27) one has for all $z \in \mathbb{R}^{2d}$

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

By the chain rule,

$$\|(\partial_z R_0)(\zeta, z)\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})} = \|\big(R_0(\zeta)(\partial_z H_0) R_0(\zeta)\big)(z)\|_{\mathcal{B}(\mathcal{H}_\mathrm{f})}\,. \tag{37}$$

Since $\partial_z H_0\, R_0(\zeta)$ is a τ-equivariant $\mathcal{B}(\mathcal{H}_\mathrm{f})$-valued symbol, its norm is periodic. Therefore it suffices to estimate its norm for $z \in B \times \mathbb{R}^d$, which yields the required bound. For a general $\alpha \in \mathbb{N}^{2d}$, the norm of $\partial^\alpha_z R_0(\zeta)$ can be bounded in a similar way. This proves that $R_0(\zeta)$ belongs to $S^1_\tau(\mathcal{B}(\mathcal{H}_\mathrm{f}))$ uniformly in ζ.

On the other hand

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

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

$$\begin{aligned}
\|(\partial_z R_0)(\zeta, z)\|_{\mathcal{B}(\mathcal{H}_\mathrm{f},\mathcal{D})} &= \|\big(R_0(\zeta)(\partial_z H_0) R_0(\zeta)\big)(z)\|_{\mathcal{B}(\mathcal{H}_\mathrm{f},\mathcal{D})} \\
&\leq C(1+k^2)\,.
\end{aligned}$$

Higher order derivatives, are bounded by the same argument, yielding that $R_0(\zeta)$ belongs to $S^w_\tau(\mathcal{B}(\mathcal{H}_\mathrm{f}, \mathcal{D}))$ uniformly in ζ. This concludes the induction argument.

From the previous argument it follows moreover that

$$\|(\partial^\alpha_z R_j)(\zeta, z)\|_{\mathcal{B}(\mathcal{H}_\mathrm{f},\mathcal{D})} \leq C_{\alpha j}\; w(z) \quad \forall\; z \in \mathcal{U}_{z_0},\; \zeta \in \Lambda(z_0) \tag{38}$$

with $C_{\alpha j}$ independent of $z_0 \in \mathbb{R}^{2d}$. By (34), this implies $\pi \in M^w_\tau(\varepsilon, \mathcal{B}(\mathcal{H}_\mathrm{f}, \mathcal{D}))$ and concludes the proof. $\square$

Proof of Proposition 8. From the projector constructed in Lemma 9 one obtains, by resummation, a semiclassical symbol $\pi \in S^1_\tau(\varepsilon, \mathcal{H}_{\mathrm{f}})$ whose asymptotic expansion is given by $\sum_{j\geq 0} \varepsilon^j \pi_j$. Then according to Proposition 26 Weyl quantization yields a bounded operator $\widehat{\pi} \in \mathcal{B}(\mathcal{H}_\tau)$, which is approximately a projector in the sense that

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

We notice that Proposition 25 implies that $H \,\widetilde{\sharp}\, \pi \in S^{w^2}_\tau(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$. But τ-equivariance implies that the norm is periodic and then $H \,\widetilde{\sharp}\, \pi$ belongs to $S^1_\tau(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$. Then $\pi \,\widetilde{\sharp}\, H = \big(H \,\widetilde{\sharp}\, \pi\big)^*$ belongs to the same class, so that $[H, \pi]_{\widetilde{\sharp}} \in S^1_\tau(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$. This *a priori* information on the symbol class, together with Lemma 9.(iii), assures that

$$[\widehat{H}, \widehat{\pi}] = \mathcal{O}_0(\varepsilon^\infty) \tag{39}$$

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

In order to get a true projector, we proceed as in [NeSo]. For ε small enough, let

$$\Pi := \frac{\mathrm{i}}{2\pi} \int_{|\zeta - 1| = \frac{1}{2}} \mathrm{d}\zeta \, (\widehat{\pi} - \zeta)^{-1} . \tag{40}$$

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

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

□

3.2 The intertwining unitaries

After we determined the decoupled subspace associated with an isolated group of bands, we aim at an effective description of the dynamics inside this subspace. In order to get a nice and workable formulation of the effective dynamics, it is convenient to map the decoupled subspace to a simpler reference space. The natural reference Hilbert space for the effective dynamics is $\mathcal{K} := L^2(\mathbb{T}^d) \otimes \mathbb{C}^\ell$ with $\ell := \dim P_{\mathcal{I}}(k)$. Notation will be simpler in the following, if we think of the fibre $\mathbb{C}^\ell$ as a subspace of $\mathcal{H}_{\mathrm{f}}$. In order to construct such a unitary mapping, we reformulate Assumption (A_2).

Assumption ($\mathbf{A}_2'$). *Let $\{E_n(k)\}_{n\in\mathcal{I}}$ be an isolated group of bands and let $\pi_{\mathrm{r}} \in \mathcal{B}(\mathcal{H}_{\mathrm{f}})$ be an orthogonal projector with $\dim \pi_{\mathrm{r}} = \ell$. There is a unitary-operator-valued map $u_0 : \mathbb{R}^{2d} \to \mathcal{U}(\mathcal{H}_{\mathrm{f}})$ so that*

$$u_0(k, r) \, \pi_0(k, r) \, u_0^*(k, r) = \pi_{\mathrm{r}} \tag{41}$$

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

$$u_0(k + \gamma^*, r) = u_0(k, r) \tau(\gamma^*)^{-1} , \tag{42}$$

and u_0 belongs to $S^1(\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$. ♢

Clearly,

$$u_0^*(k+\gamma^*,r)=\tau(\gamma^*)u_0^*(k,r). \tag{43}$$

An operator-valued symbol satisfying (43) (resp. (42)) is called left τ-covariant (resp. right τ-covariant).

The equivalence of (A_2) and (A_2') can be seen as follows. According to Assumption (A_2), there exists an orthonormal basis $\{\psi_j(k)\}_{j=1}^{\ell}$ of $\mathrm{Ran}P_{\mathcal{I}}(k)$ which is smooth and τ-equivariant with respect to k. Let $\pi_{\mathrm{r}}:=\pi_0(k_0,r_0)$ for any fixed point (k_0,r_0). By the gap condition, $\dim\pi_{\mathrm{r}}=\dim P_{\mathcal{I}}(k)$. Then for any orthonormal basis $\{\chi_j\}_{j=1}^{\ell}$ for $\mathrm{Ran}\pi_{\mathrm{r}}$, the formula

$$\widetilde{u}_0(k,r):=\sum_{j=1}^{\ell}|\chi_j\rangle\,\langle\psi_j(k-A(r))| \tag{44}$$

defines a partial isometry which can be extended to a unitary operator $u_0(k,r)\in\mathcal{U}(\mathcal{H}_{\mathrm{f}})$. The fact that $\{\psi_j(k)\}_{j=1}^{\ell}$ spans $\mathrm{Ran}P_{\mathcal{I}}(k)$ implies (41), and the τ-equivariance of $\psi_j(k)$ reflects in (42).

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

$$\psi_j(k-A(r)):=u_0^*(k,r)\chi_j,$$

with $\{\chi_j\}_{j=1}^{\ell}$ spanning $\mathrm{Ran}\pi_{\mathrm{r}}$, defines an orthonormal basis for $\mathrm{Ran}P_{\mathcal{I}}(k)$ which satisfies Assumption (A_2).

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

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

As in [PST_1] we introduce the orthogonal projector $\Pi_{\mathrm{r}}:=\hat{\pi}_{\mathrm{r}}\in\mathcal{B}(\mathcal{H}_{\mathrm{ref}})$ since the effective intraband dynamics can be described in

$$\mathcal{K}:=\mathrm{Ran}\Pi_{\mathrm{r}}\cong L^2_{\tau\equiv\mathbf{1}}(\mathbb{R}^d,\mathbb{C}^\ell)\cong L^2(\mathbb{T}^d,\mathbb{C}^\ell)$$

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

Proposition 10. *Let $\{E_n\}_{n\in\mathcal{I}}$ be an isolated group of bands, see Definition 4, and let Assumptions* (A_1) *and* (A_2') *be satisfied. Then there exists a unitary operator $U:\mathcal{H}_\tau\to\mathcal{H}_{\mathrm{ref}}$ such that*

$$U\,\Pi\,U^*=\Pi_{\mathrm{r}} \tag{45}$$

and $U=\hat{u}+\mathcal{O}_0(\varepsilon^\infty)$, where $u\asymp\sum_{j\geq0}\varepsilon^j u_j$ belong to $S^1(\varepsilon,\mathcal{B}(\mathcal{H}_{\mathrm{f}}))$, is right τ-covariant at any order and has principal symbol u_0.

Proof. Since u_0 is right τ-covariant, one proves by induction that the same holds true for any u_j. Indeed, by referring to the notation in [PST$_1$], one has that

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

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

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

and the induction hypothesis, it follows that A_{n+1} is a periodic symbol. Then $w^{(n)} := u^{(n)} + \varepsilon^{n+1} a_{n+1} u_0$ is right τ-covariant. Then the defining equation

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

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

One notices that right τ-covariance is nothing but a special case of (τ_1, τ_2)-equivariance, for $\tau_2 \equiv \mathbf{1}$ and $\tau_1 = \tau$. Thus it follows from Proposition 26 that the Weyl quantization of u is a bounded operator $\widehat{u} \in \mathcal{B}(\mathcal{H}_\tau, \mathcal{H}_{\mathrm{ref}})$ such that:

(i) $\widehat{u}\, \widehat{u}^* = \mathbf{1}_{\mathcal{H}_{\mathrm{ref}}} + \mathcal{O}_0(\varepsilon^\infty)$ and $\widehat{u}^* \widehat{u} = \mathbf{1}_{\mathcal{H}_\tau} + \mathcal{O}_0(\varepsilon^\infty)$,

(ii) $\widehat{u}\, \Pi\, \widehat{u}^* = \Pi_{\mathrm{r}} + \mathcal{O}_0(\varepsilon^\infty)$.

Finally we modify $\widehat{u}$ as in [PST$_1$] by an $\mathcal{O}_0(\varepsilon^\infty)$-term in order to get the unitary operator $U \in \mathcal{U}(\mathcal{H}_\tau, \mathcal{H}_{\mathrm{ref}})$. □

3.3 The effective Hamiltonian

The final step in space-adiabatic perturbation theory is to define and compute the effective Hamiltonian for the intra-band dynamics. This is done, in principle, by projecting the full Hamiltonian $H^\varepsilon_{\mathrm{BF}}$ to the decoupled subspace and afterwards rotating to the reference space.

Proposition 11. *Let $\{E_n\}_{n\in\mathcal{I}}$ be an isolated group of bands and let Assumptions (A_1) and (A_2) be satisfied. Let h be a resummation in $S^1_{\tau\equiv\mathbf{1}}(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))$ of the formal symbol*

$$h = u \sharp \pi \sharp H \sharp \pi \sharp u^* \in M^1_{\tau\equiv\mathbf{1}}(\varepsilon, \mathcal{B}(\mathcal{H}_{\mathrm{f}}))\,. \tag{46}$$

Then $\widehat{h} \in \mathcal{B}(\mathcal{H}_{\mathrm{ref}})$, $[\widehat{h}, \Pi_{\mathrm{r}}] = 0$ and

$$\big(\mathrm{e}^{-\mathrm{i} H^\varepsilon_{\mathrm{BF}} t} - U^* \,\mathrm{e}^{-\mathrm{i}\widehat{h} t}\, U\big)\Pi = \mathcal{O}_0(\varepsilon^\infty(1 + |t|))\,. \tag{47}$$

Remark 12. The definition of the effective Hamiltonian is not entirely unique in the sense that any H_{eff} satisfying (47) would serve as well as an effective Hamiltonian. However, the asymptotic expansion of H_{eff} is unique and therefore it is most convenient to define the effective Hamiltonian through (46). ◊

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

First note that (46) follows from the following facts: according to Lemma 9 and Proposition 25 we have that

$$\pi \,\sharp\, H \,\sharp\, \pi \in M^{w^2}_\tau(\varepsilon, \mathcal{B}(\mathcal{H}_{\rm f})) = M^1_\tau(\varepsilon, \mathcal{B}(\mathcal{H}_{\rm f}))\,,$$

where we used that τ is a unitary representation. With Proposition 10 it follows that $h \in M^1_{\tau\equiv 1}(\varepsilon, \mathcal{B}(\mathcal{H}_{\rm f}))$. Therefore $\widehat{h} \in \mathcal{B}(\mathcal{H}_{\rm ref})$ follows from Proposition 26, while $[\widehat{h}, \Pi_{\rm r}] = 0$ is satisfied by construction.

It remains to check (47):

$$\begin{aligned}\big(\mathrm{e}^{-\mathrm{i}\widehat{H}t} - U^*\,\mathrm{e}^{-\mathrm{i}\widehat{h}t}\,U\big)\Pi &= \big(\mathrm{e}^{-\mathrm{i}\widehat{H}t} - \mathrm{e}^{-\mathrm{i}U^*\,\widehat{h}\,Ut}\big)\widehat{\pi} + \mathcal{O}_0(\varepsilon^\infty)\\ &= \big(\mathrm{e}^{-\mathrm{i}\widehat{\pi}\widehat{H}\widehat{\pi}t} - \mathrm{e}^{-\mathrm{i}U^*\,\widehat{h}\,Ut}\big)\widehat{\pi} + \mathcal{O}_0(\varepsilon^\infty)\\ &= \mathcal{O}(\varepsilon^\infty(1+|t|))\,,\end{aligned}$$

where the last equality follows from the usual Duhammel argument and the fact that the difference of the generators is $\mathcal{O}_0(\varepsilon^\infty)$ in the norm of bounded operators by construction. □

Since $[\widehat{h}, \Pi_{\rm r}] = 0$, the effective Hamiltonian will be regarded, without differences in notation, either as an element of $\mathcal{B}(\mathcal{H}_{\rm ref})$ or as an element of $\mathcal{B}(\mathcal{K})$.

We now compute the principal and the subprincipal symbol of $\widehat{h}$ for the special but most relevant case of an isolated ℓ-fold degenerate eigenvalue, i.e. $E_n(k) \equiv E(k)$ for every $n \in \mathcal{I}$, $|\mathcal{I}| = \ell$. Recall that in this special case Assumption (A_2) is equivalent to the existence of an orthonormal system of smooth and τ-equivariant Bloch functions corresponding to the eigenvalue $E(k)$. If $\ell = 1$ then Assumption (A_2) is always satisfied. The part of u_0 intertwining π_0 and $\pi_{\rm r}$ is given by equation (44) where $\psi_j(k)$ are now Bloch functions, i.e. eigenvectors of $H_{\rm per}(k)$ to the eigenvalue $E(k)$.

Proof of Corollary 6. In the following h is identified with $\pi_{\rm r} h \pi_{\rm r}$ and regarded as a $\mathcal{B}(\mathbb{C}^\ell)$-valued symbol. We consider the matrix elements

$$h(k,r)_{\alpha\beta} := \langle \chi_\alpha, h(k,r)\chi_\beta\rangle$$

for $\alpha, \beta \in \{1, \ldots, \ell\}$, where we recall that $\chi_\alpha = u_0(k,r)\psi_\alpha(k - A(r))$. Equation (21) follows immediately from the fact that $h_0 = u_0\, H_0\, u_0^*$ and that ψ_α are Bloch functions. As for h_1, we use the general formula of [PST_1], which reads applied to the present setting as

$$\begin{aligned} h_{1\,\alpha\beta}(k,r) &= -\mathrm{i}\,\big\langle \psi_\alpha(\widetilde{k}),\, \{E(\widetilde{k}) + \phi(r), \psi_\beta(\widetilde{k})\}\big\rangle\\ &\quad - \tfrac{\mathrm{i}}{2}\big\langle \psi_\alpha(\widetilde{k}), \{(H_{\rm per}(\widetilde{k}) - E(\widetilde{k})), \psi_\beta(\widetilde{k})\}\big\rangle\,. \end{aligned} \qquad (48)$$

Here $\{A, \varphi\} = \nabla_r A \cdot \nabla_k \varphi - \nabla_k A \cdot \nabla_r \varphi$ are the Poisson brackets for an operator-valued function $A(k,r)$ acting on a vector-valued function $\varphi(k,r)$. We need to evaluate (48). Inserting (44) and performing a straightforward computation the first term in (48) gives the first term in (22) while the second term contributes to the $\alpha\beta$ matrix element with

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

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

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

since ψ_α is in the kernel of $(H_{\mathrm{per}} - E)$. Finally the imaginary part of

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

vanishes, as can be seen by direct computation, concluding the proof. □

4 Semiclassical dynamics for Bloch electrons

Up to now we approximated the full quantum mechanical time-evolution generated by (5) by a quantum mechanical time-evolution on a smaller Hilbert space and with the effective Hamiltonian $\widehat{h}$ as a simpler generator. The effective Hamiltonian is, in general, a pseudodifferential operator with a matrix-valued symbol. Whenever the isolated group of bands under consideration contains just a single eigenvalue of multiplicity ℓ, then its principal symbol is a scalar multiple of the identity. It is well known, as discussed e.g. in [PST$_1$], how to perform the semiclassical limit for such Hamiltonians.

In this section we take a slightly different attitude and show how to incorporate the first order correction into the ε-dependent classical flow generated by the dynamical equations (4). This program is performed in two steps. We first prove an Egorov theorem for observables in the reference representation and then, in order to obtain the result for the physical observables in Theorem 2, we translate the results from the reference representation on $\mathcal{H}_{\mathrm{ref}}$ back to the original representation on $L^2(\mathbb{R}^d)$. The latter task turns out to be computationally quite involved. However, since the beautiful equations (4) are new, with predecessors in [SuNi], and since it is not obvious how to base their derivation on WKB techniques, see [DGR], we provide the details of the computation.

For the same reason it is worthwhile, before performing this program, to show that the semiclassical equations (4) are Hamiltonian equations with respect to a suitable symplectic structure. The Hamiltonian formulation has the advantage that the existence of global solutions of (4) follows immediately, and that it becomes straightforward to deal with questions related to symmetries and conserved quantities.

The dynamical equations (4), which define the ε-corrected semiclassical model, are given by

$$\begin{aligned} \dot{q} &= \nabla_v H_{\rm sc}(q,v) - \varepsilon\, \dot{v} \times \Omega_n(v)\,, \\ \dot{v} &= -\nabla_q H_{\rm sc}(q,v) + \dot{q} \times B(q) \end{aligned} \tag{49}$$

with Hamiltonian

$$H^{\varepsilon}_{\rm sc}(q,v) = E_n(v) + \phi(q) - \varepsilon\, M_n(v)\cdot B(q).$$

Recall that we are using the notation introduced in Remark 7 and that B and Ω_n are the 2-forms corresponding to the magnetic field and to the curvature of the Berry connection, i.e. in components

$$B(q)_{ij} = \big(\partial_i A_j - \partial_j A_i\big)(q)$$

for $i,j \in \{1,\dots,d\}$, and

$$\Omega_n(v)_{ij} = \big(\partial_i \mathcal{A}_j - \partial_j \mathcal{A}_i\big)(v)\,.$$

Let us fix a system of coordinates $z = (q,v)$ in $\mathbb{R}^{2d}$. The standard symplectic form $\Theta_0 = \Theta_0(z)_{lm}\; dz_m \wedge dz_l$, where $l,m \in \{1,\dots,2d\}$, has coefficients given by the constant matrix

$$\Theta_0(z) = \begin{pmatrix} 0 & -\mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix},$$

where $\mathbb{I}$ is the identity matrix in $\mathrm{Mat}(d,\mathbb{R})$. The symplectic form, which turns (49) into Hamilton's equation of motion for $H_{\rm sc}$, is given by the 2-form $\Theta_{B,\,\varepsilon} = \Theta_{B,\,\varepsilon}(z)_{lm}\; dz_m \wedge dz_l$ with coefficients

$$\Theta_{B,\,\varepsilon}(q,v) = \begin{pmatrix} B(q) & -\mathbb{I} \\ \mathbb{I} & \varepsilon\;\Omega_n(v) \end{pmatrix}. \tag{50}$$

For $\varepsilon = 0$ the 2-form $\Theta_{B,\,\varepsilon}$ coincides with the magnetic symplectic form Θ_B usually employed to describe in a gauge-invariant way the motion of a particle in a magnetic field ([MaRa], Section 6.6). For ε small enough, the matrix (50) defines a symplectic form, i.e. a closed non-degenerate 2-form. Indeed, since $\det \Theta_B = 1$ it follows that, for ε small enough, $\Theta_{B,\,\varepsilon}$ is not degenerate. In particular it is sufficient to choose

$$\varepsilon < \sup_{q,v\in\mathbb{R}^d} \big(\|B(q)\,\Omega_n(v)\| + \|\Omega_n(v)\|\big).$$

The closedness of $\Theta_{B,\,\varepsilon}$ follows from the fact that B and Ω_n correspond to closed 2-forms over $\mathbb{R}^d$.

With these definitions the corresponding Hamiltonian equations are

$$\Theta_{B,\,\varepsilon}(z)\; \dot{z} = \mathrm{d}H_{\rm sc}(z)\,,$$

or equivalently

$$\begin{pmatrix} B(q) & -\mathbb{I} \\ \mathbb{I} & \varepsilon\, \Omega_n(v) \end{pmatrix} \begin{pmatrix} \dot q \\ \dot v \end{pmatrix} = \begin{pmatrix} \nabla_q H(q,v) \\ \nabla_v H(q,v) \end{pmatrix},$$

which agrees with (49). We notice that our discussion remains valid if Ω_n admits a potential only locally, as it happens generically for magnetic Bloch bands.

We now turn to the derivation of the semiclassical model (4). Hence we assume that the isolated group of bands consists of a single non-degenerate Bloch band $E(k)$. We start with Egorov's theorem for observables in the reference space. As the only difference to the standard presentation of Egorov's theorem, as e.g. in [Ro], we treat the first order corrections by considering an ε-dependent Hamiltonian flow instead of having a separate dynamics for the subprincipal symbol of an observable.

Proposition 13. *Let E be a simple isolated Bloch band and let $\widehat{h}$ be the effective Hamiltonian constructed in Theorem 5, which acts on the reference space $\mathcal{K} = L^2_{\tau\equiv 1}(\mathbb{R}^d)$ of Γ^*-periodic L^2_{loc}-functions. Let $\widetilde{\Phi}^t : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ be the Hamiltonian flow generated by the Hamiltonian function*

$$h_{\mathrm{cl}}(k,r) = h_0(k,r) + \varepsilon h_1(k,r)\,.$$

Then for any semiclassical observable $\widehat{a} = a_0(k, \mathrm{i}\varepsilon\nabla_k) + \varepsilon a_1(k, \mathrm{i}\varepsilon\nabla_k)$ with $a \in S^1(\varepsilon, \mathbb{C})$ we have that

$$\left\| \,\mathrm{e}^{\mathrm{i}\widehat{h}t/\varepsilon}\, \widehat{a}\, \mathrm{e}^{-\mathrm{i}\widehat{h}t/\varepsilon} - \widehat{a \circ \widetilde{\Phi}^t}\, \right\| = \mathcal{O}(\varepsilon^2) \tag{51}$$

uniformly for any finite interval in time.

Proof. Since the Hamiltonian function is bounded with bounded derivatives, it follows immediately that $a \circ \widetilde{\Phi}^t \in S^1(\varepsilon)$ and that $\frac{\mathrm{d}}{\mathrm{d}t}(a \circ \widetilde{\Phi}^t) \in S^1(\varepsilon)$. Therefore the proof is just the standard computation

$$\begin{aligned} \mathrm{e}^{\mathrm{i}\widehat{h}t/\varepsilon}\, \widehat{a}\, \mathrm{e}^{-\mathrm{i}\widehat{h}t/\varepsilon} - \widehat{a \circ \widetilde{\Phi}^t} &= \int_0^t \mathrm{d}t' \, \frac{\mathrm{d}}{\mathrm{d}t'} \left(\mathrm{e}^{\mathrm{i}\widehat{h}t'/\varepsilon} \left(\widehat{a \circ \widetilde{\Phi}^{t-t'}} \right) \mathrm{e}^{-\mathrm{i}\widehat{h}t'/\varepsilon} \right) \\ = \quad \int_0^t \mathrm{d}t' \, \mathrm{e}^{\mathrm{i}\widehat{h}t'/\varepsilon} & \left(\frac{\mathrm{i}}{\varepsilon} \left[\widehat{h}, \left(\widehat{a \circ \widetilde{\Phi}^{t-t'}}\right) \right] - \left(\tfrac{\mathrm{d}}{\mathrm{d}t'} \left(a \circ \widetilde{\Phi}^{t-t'} \right) \right)^{\widehat{}} \right) \mathrm{e}^{-\mathrm{i}\widehat{h}t'/\varepsilon}\,, \end{aligned}$$

together with the fact that the integrand is $\mathcal{O}(\varepsilon^2)$ in the norm of bounded operators, since by construction

$$\frac{\mathrm{d}}{\mathrm{d}t'} (a \circ \widetilde{\Phi}^{t-t'}) = \left\{ h_{\mathrm{cl}},\, a \circ \widetilde{\Phi}^{t-t'} \right\}$$

and, computing the expansion of the Moyal product,

$$\frac{\mathrm{i}}{\varepsilon} \left[h, a \circ \widetilde{\Phi}^{t-t'} \right]_{\widetilde{\sharp}} = \left\{ h_{\mathrm{cl}},\, a \circ \widetilde{\Phi}^{t-t'} \right\} + \mathcal{O}(\varepsilon^2)\,.$$

∎

In order to obtain the Egorov theorem for the physical observables, we need to undo the transformation to the reference space and the Bloch-Floquet transformation. We start with the simpler observation on how the Bloch-Floquet transformation maps semiclassical observables.

Proposition 14. *Let $a \in S^1(\varepsilon, \mathbb{C})$ be Γ^*-periodic, i.e. $a(q, p+\gamma^*) = a(q,p)$ for all $\gamma^* \in \Gamma^*$. Let $b(k,r) = a(r,k)$ then $b \in S^1_\tau(\varepsilon, \mathbb{C})$ and*

$$\widehat{a} = \mathcal{U}^* \,\widehat{b}\,\mathcal{U}\,,$$

where the Weyl quantization is in the sense of $\widehat{a} = a(\varepsilon x, -\mathrm{i}\nabla_x)$ acting on $L^2(\mathbb{R}^d)$ and $\widehat{b} = b(k, \varepsilon \mathrm{i}\nabla_k)$ acting on $\mathcal{H}_\tau$.

Remark 15. An analogous statement *cannot* be true for general operator-valued τ-equivariant symbols. For example, the symbol $b(k,r) := H_{\mathrm{per}}(k - A(r))$ is τ-equivariant and in particular a semiclassical observable. However, the corresponding operator in the original representation is

$$\mathcal{U}^* \,\widehat{b}\,\mathcal{U} = -\frac{1}{2}\big(-\mathrm{i}\nabla_x - A(\varepsilon x)\big)^2 + V_\Gamma(x)$$

which cannot be written as a ε-pseudodifferential operator with scalar symbol. $\diamondsuit$

Proof. We give the proof for $a(\cdot, p) \in \mathcal{S}(\mathbb{R}^d)$. The general result follows from standard density arguments, cf. [DiSj]. For $\psi \in \mathcal{S}(\mathbb{R}^d)$ we have according to (65) the explicit formula

$$\big(a(\varepsilon x, -\mathrm{i}\nabla_x)\psi\big)(x) = \frac{1}{(2\pi)^{d/2}} \sum_{\gamma\in\Gamma} \int_{\mathbb{R}^d} \mathrm{d}\eta \big(\mathcal{F}a\big)(\eta,\gamma)\ \mathrm{e}^{\mathrm{i}\varepsilon(\eta\cdot\gamma)/2} \mathrm{e}^{\mathrm{i}\varepsilon\eta\cdot x} \psi(x+\gamma)\,. \tag{52}$$

On the other hand for $(\mathcal{U}\psi)(k,r) =: \varphi(k,r)$ by definition it holds that

$$\big(b(k, \mathrm{i}\varepsilon\nabla_k)\varphi\big)(k,r) = \sum_{\gamma\in\Gamma} \int_{\mathbb{R}^d} \mathrm{d}\eta \big(\mathcal{F}b\big)(\gamma,\eta)\ \mathrm{e}^{-\mathrm{i}\varepsilon(\eta\cdot\gamma)/2} \mathrm{e}^{\mathrm{i}\gamma\cdot k} \varphi(k - \varepsilon\eta, r)\,. \tag{53}$$

The assumptions on a and ψ guarantee that all the integrals and sums in the following expressions are absolutely convergent and thus that interchanges in the order of integration are justified by Fubini's theorem.

We compute the inverse Bloch-Floquet transform of (53) using (11),

$$\begin{aligned}
&\big(\mathcal{U}^{-1}\widehat{b}\,\varphi\big)(x) = \qquad\qquad (54)\\
&= \sum_{\gamma\in\Gamma} \int_B \mathrm{d}k \int_{\mathbb{R}^d} \mathrm{d}\eta\ \big(\mathcal{F}b\big)(\gamma,\eta)\ \mathrm{e}^{\mathrm{i}k\cdot x} \mathrm{e}^{-\mathrm{i}\varepsilon(\eta\cdot\gamma)/2} \mathrm{e}^{\mathrm{i}\gamma\cdot k} \varphi(k-\varepsilon\eta, [x])\\
&= \sum_{\gamma\in\Gamma} \int_{\mathbb{R}^d} \mathrm{d}\eta\ \big(\mathcal{F}b\big)(\gamma,\eta) \mathrm{e}^{\mathrm{i}\varepsilon(\eta\cdot\gamma)/2} \mathrm{e}^{\mathrm{i}\varepsilon\eta\cdot x} \int_B \mathrm{d}k\, \mathrm{e}^{\mathrm{i}(k-\varepsilon\eta)\cdot(x+\gamma)} \varphi(k-\varepsilon\eta, [x])\,.
\end{aligned}$$

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

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

Inserting this expression in the last line of (54) and comparing with (52) concludes the proof. $\square$

Before we arrive at the proof of Theorem 2, we must also understand how the unitary map constructed in Section 3.2 maps observables in the Bloch-Floquet representation to observables in the reference representation.

Proposition 16. *Let $\widehat{b} = b_0(k,\varepsilon\mathrm{i}\nabla_k) + \varepsilon\, b_1(k,\varepsilon\mathrm{i}\nabla_k)$ with symbol $b \in S^1(\varepsilon,\mathbb{C})$ which is Γ^*-periodic in the first argument. Let $U : \Pi\mathcal{H}_\tau \to \mathcal{K}$ be the unitary map constructed in Section 3.2. Then*

$$U\,\Pi\,\widehat{b}\,\Pi\,U^* = \widehat{c} + \mathcal{O}(\varepsilon^2)\,,$$

where $c(\varepsilon,k,r) = \big(b\circ T\big)(k,r)$ with

$$T:\mathbb{R}^{2d}\to\mathbb{R}^{2d}\,,\quad (k,r)\mapsto \Big(k+\varepsilon\,\mathcal{A}_m\big(k-A(r)\big)\nabla A_m(r),\; r+\varepsilon\mathcal{A}\big(k-A(r)\big)\Big)\,.$$

Here and in the following summation over indices appearing twice is implicit.

Proof. In order to compute $c = u\,\sharp\,\pi\,\sharp\,b\,\sharp\,\pi\,\sharp\,u^*$, observe that, since b is scalar-valued, the principal symbol remains unchanged, i.e. $c_0 = u_0\,\pi_0\,b_0\,\pi_0\,u_0^* = b_0$. For the subprincipal symbol we use the general transformation formula (48) obtained for the Hamiltonian, which applies to all operators whose principal symbol commutes with π_0. In this case the eigenvalue E in (48) must be replaced by the corresponding principal symbol and a term for the subprincipal symbol b_1 must be added, cf. [PST$_1$]. Hence we find that

$$\begin{aligned} c_1(k,r) &= -\mathrm{i}\,\big\langle\psi(k-A(r)),\{b_0(k,r),\psi(k-A(r))\}\big\rangle \\ &\quad + \langle\psi(k-A(r)),b_1(k,r)\psi(k-A(r))\rangle \\ &= \partial_{k_n}b_0(k,r)\,\mathrm{i}\,\big\langle\psi(k-A(r)),\partial_m\psi(k-A(r))\big\rangle\,\partial_n A_m(r) \\ &\quad + \partial_{r_n}b_0(k,r)\,\mathrm{i}\,\big\langle\psi(k-A(r)),\partial_n\psi(k-A(r))\big\rangle + b_1(k,r) \\ &= \partial_{k_n}b_0(k,r)\,\mathcal{A}_m(k-A(r))\,\partial_n A_m(r) \\ &\quad + \partial_{r_n}b_0(k,r)\,\mathcal{A}_n(k-A(r)) + b_1(k,r)\,, \end{aligned}$$

where summation over indices appearing twice is implicit. Now a comparison with the Taylor expansion of $\big(b\circ T\big)(k,r)$ in powers of ε proves the claim. $\square$

We have now all the ingredients needed for the

Proof of Theorem 2. Let $a \in C_{\rm b}^\infty(\mathbb{R}^{2d})$ be Γ^*-periodic in the second argument, then according to Proposition 14 we have

$$\Pi_n^\varepsilon \, \mathrm{e}^{\mathrm{i}H^\varepsilon t/\varepsilon} \, \widehat{a} \, \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} \, \Pi_n^\varepsilon = \mathcal{U}^* \, \Pi \, \mathrm{e}^{\mathrm{i}H^\varepsilon_{\rm BF} t/\varepsilon} \, \widehat{b} \, \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm BF} t/\varepsilon} \, \Pi \mathcal{U} \tag{55}$$

with $b(k,r) = a(r,k)$. With Theorem 5 and Proposition 16 we find that

$$\Pi \, \mathrm{e}^{\mathrm{i}H^\varepsilon_{\rm BF} t/\varepsilon} \, \widehat{b} \, \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm BF} t/\varepsilon} \, \Pi = U^* \, \mathrm{e}^{\mathrm{i}\widehat{h} t/\varepsilon} \, \widehat{c} \, \mathrm{e}^{-\mathrm{i}\widehat{h} t/\varepsilon} \, U + \mathcal{O}(\varepsilon^2) \,, \tag{56}$$

where $c(\varepsilon, k, r) = \big(b \circ T\big)(k,r)$. Now we can apply Proposition 13 to conclude that

$$\mathrm{e}^{\mathrm{i}\widehat{h} t/\varepsilon} \, \widehat{c} \, \mathrm{e}^{-\mathrm{i}\widehat{h} t/\varepsilon} = \widehat{\big(c \circ \widetilde{\Phi}^t\big)} + \mathcal{O}(\varepsilon^2).$$

Since, for ε sufficiently small, T is a diffeomorphism, we can write

$$c \circ \widetilde{\Phi}^t = c \circ T^{-1} \circ T \circ \widetilde{\Phi}^t \circ T^{-1} \circ T =: c \circ T^{-1} \circ \overline{\Phi}^t \circ T = b \circ \overline{\Phi}^t \circ T \,,$$

where the flow $\overline{\Phi}^t_\varepsilon$ in the new coordinates will be computed explicitly below. Inserting the results into (56), we obtain

$$\begin{aligned} \Pi \, \mathrm{e}^{\mathrm{i}H^\varepsilon_{\rm BF} t/\varepsilon} \, \widehat{b} \, \mathrm{e}^{-\mathrm{i}H^\varepsilon_{\rm BF} t/\varepsilon} \, \Pi &= U^* \, \widehat{\big(b \circ \overline{\Phi}^t \circ T\big)} \, U + \mathcal{O}(\varepsilon^2) \\ &= \Pi \, \widehat{\big(b \circ \overline{\Phi}^t\big)} \, \Pi + \mathcal{O}(\varepsilon^2) \,, \end{aligned}$$

where we used Proposition 16 for the second equality. Inserting into (55) we finally find that

$$\Pi_n^\varepsilon \, \mathrm{e}^{\mathrm{i}H^\varepsilon t/\varepsilon} \, \widehat{a} \, \mathrm{e}^{-\mathrm{i}H^\varepsilon t/\varepsilon} \, \Pi_n^\varepsilon = \Pi_n^\varepsilon \, \widehat{\big(a \circ \overline{\Phi}^t\big)} \, \Pi_n^\varepsilon + \mathcal{O}(\varepsilon^2) \,, \tag{57}$$

where we did not make the exchange of the order of the arguments in a explicit.

Since we can compute the flow only approximately and only through its vector field, we make use of the following lemma.

Lemma 17. *Let $\Phi_i : \mathbb{R}^{2d} \times \mathbb{R} \to \mathbb{R}^{2d}$ be the flow associated with the vector field $v_i \in C_{\rm b}^\infty(\mathbb{R}^{2d}, \mathbb{R}^{2d})$, $i = 1,2$.*

(i) *If for all $\alpha \in \mathbb{N}^{2d}$ there is a $c_\alpha < \infty$ such that*

$$\sup_{x \in \mathbb{R}^{2d}} |\, \partial^\alpha \, (v_1 - v_2)(x)| \leq c_\alpha \, \varepsilon^2 \,,$$

then for each bounded interval $I \subset \mathbb{R}$ there are constants $C_{I,\alpha} < \infty$ such that

$$\sup_{t \in I, x \in \mathbb{R}^{2d}} |\, \partial^\alpha \, (\Phi_1^t - \Phi_2^t)(x)| \leq C_{I,\alpha} \, \varepsilon^2 \,. \tag{58}$$

(ii) *Let $a \in S^1(\varepsilon, \mathbb{C})$. If (58) holds for the flows Φ_1, Φ_2, then there is a constant $C < \infty$, such that for all $t \in I$*

$$\big\| \, \widehat{a \circ \Phi_1^t} - \widehat{a \circ \Phi_2^t} \, \big\|_{\mathcal{B}(L^2(\mathbb{R}^d))} \leq C \, \varepsilon^2 \,.$$

Proof. Assertion (i) is just a simple application of Gronwall's lemma. Assertion (ii) follows from the fact that the norm of the quantization of a symbol in S^1 is bounded by a constant times the sup-norm of finitely many derivatives of the symbol, which are $\mathcal{O}(\varepsilon^2)$ according to (58). $\square$

According to assertion (ii) of the lemma it suffices to show that

$$\overline{\Phi}^t(q,p) = \Big(\Phi^t_{n\,q}(q, p - A(q)),\ \Phi^t_{n\,v}(q, p - A(q)) + A(q)\Big) + \mathcal{O}(\varepsilon^2)$$

in the above sense, where Φ^t_n is the flow of (4). And from assertion (i) we infer that it suffices to prove the analogous properties on the level of the vector fields.

Through a subsequent change of coordinates we aim at computing the vector field of Φ^t_n up to an error of order $\mathcal{O}(\varepsilon^2)$. We start with the vector field of $\widetilde{\Phi}^t$. The effective Hamiltonian on the reference space including first order terms reads

$$\begin{aligned} h(r,k) &= E(k - A(r)) + \phi(r) \\ &\quad - \varepsilon\Big(F_{\mathrm{Lor}}(r, \nabla E(k - A(r))) \cdot \mathcal{A}(k - A(r)) + B(r) \cdot M(k - A(r))\Big)\,, \end{aligned} \tag{59}$$

with the Lorentz force

$$F_{\mathrm{Lor}}(r, \nabla E(k - A(r))) = -\nabla\phi(r) + \nabla E(k - A(r)) \times B(r)\,.$$

To simplify the computation we switch to the kinetic momentum $\widetilde{k} = k - A(r)$. A straightforward computation, which is explained below, yields

$$\begin{aligned} \dot{r} &= \nabla E(\widetilde{k}) - \varepsilon \nabla_{\widetilde{k}}\Big(\mathcal{A}(\widetilde{k}) \cdot F_{\mathrm{Lor}}(r, \widetilde{k}) + B(r) \cdot M(\widetilde{k})\Big)\,, \\ \dot{\widetilde{k}} &= -\nabla\phi(r) + \dot{r} \times B(r) + \varepsilon \nabla_r\Big(\mathcal{A}(\widetilde{k}) \cdot F_{\mathrm{Lor}}(r, \widetilde{k}) + B(r) \cdot M(\widetilde{k})\Big)\,. \end{aligned} \tag{60}$$

As the next step we perform the change of coordinates induced by T,

$$q = r + \varepsilon \mathcal{A}(\widetilde{k})\,, \qquad p = \widetilde{k} - A(r) + \varepsilon \nabla_r\big(\mathcal{A}(\widetilde{k}) \cdot A(r)\big)\,, \tag{61}$$

and then switch to the kinetic momentum

$$\begin{aligned} v &= p - A(q) \\ &= \widetilde{k} + \varepsilon \mathcal{A}_l(\widetilde{k}) \nabla A_l(r) - \varepsilon \mathcal{A}_l(\widetilde{k}) \partial_l A(r) + \mathcal{O}(\varepsilon^2) \\ &= \widetilde{k} + \varepsilon\, \mathcal{A}(\widetilde{k}) \times B(r) + \mathcal{O}(\varepsilon^2)\,, \end{aligned} \tag{62}$$

where we used Taylor expansion. The inverse transformations are

$$\begin{aligned} r &= q - \varepsilon\, \mathcal{A}(v) + \mathcal{O}(\varepsilon^2)\,, \\ \widetilde{k} &= v - \varepsilon\, \mathcal{A}(v) \times B(q) + \mathcal{O}(\varepsilon^2)\,, \end{aligned}$$

which inserted into (60) yield (4).

This concludes our proof. However, since the corrected semiclassical equations (4) constitute a novel result, we supply the details of the computations skipped before. The canonical equations of motion of the Hamiltonian (59) are, componentwise,

$$\begin{aligned}\dot r_j &= \partial_{k_j} h(r,k) = \partial_{k_j} E(k-A(r)) \\ &\quad -\varepsilon\,\partial_{k_j}\Big(F_{\mathrm{Lor}}(r,k-A(r))\cdot\mathcal{A}(k-A(r)) + B(r)\cdot M(k-A(r))\Big)\,,\end{aligned}$$

$$\begin{aligned}\dot k_j = {}& -\partial_{r_j} h(r,k) = -\partial_j\phi(r) + \partial_l E(k-A(r))\partial_j A_l(r) \\ & -\varepsilon\,\partial_{k_l}\Big(\mathcal{A}(k-A(r))\cdot F_{\mathrm{Lor}}(r,k-A(r)) + B(r)\cdot M(k-A(r))\Big)\,\partial_j A_l(r) \\ & -\varepsilon\,\mathcal{A}_l(k-A(r))\Big(\partial_j\partial_l\phi(r) - \big(\nabla E(k-A(r))\times\partial_j B(r)\big)_l\Big) \\ & +\varepsilon\,\partial_j B(r)\cdot M(k-A(r))\,,\end{aligned}$$

with the convention to sum over repeated indices. Substituting $\widetilde{k} = k - A(r)$ one obtains

$$\dot r_j = \partial_j E(\widetilde{k}) - \varepsilon\,\partial_{\widetilde{k}_j}\Big(F_{\mathrm{Lor}}(r,\widetilde{k})\cdot\mathcal{A}(\widetilde{k}) + B(r)\cdot M(\widetilde{k})\Big)$$

and

$$\begin{aligned}\dot{\widetilde{k}}_j &= \dot k_j - \partial_l A_j(r)\,\dot r_l \\ &= -\partial_j\phi(r) + \partial_l E(\widetilde{k})\,\partial_j A_l(r) \\ &\quad -\varepsilon\,\partial_{k_l}\Big(\mathcal{A}(\widetilde{k})\cdot F_{\mathrm{Lor}}(r,\widetilde{k}) + M(\widetilde{k})\cdot B(r)\Big)\,\partial_j A_l(r) \\ &\quad +\varepsilon\,\mathcal{A}_l(\widetilde{k})\,\partial_{r_j} F_{\mathrm{Lor}\,l}(r,\widetilde{k}) + \varepsilon\,\partial_j B(r)\cdot M(k-A(r)) - \partial_l A_j(r)\,\dot r_l \\ &= -\partial_j\phi(r) + \dot r_l\Big(\partial_j A_l(r) - \partial_l A_j(r)\Big) \\ &\quad +\varepsilon\,\mathcal{A}_l(\widetilde{k})\,\partial_{r_j} F_{\mathrm{Lor}\,l}(r,\widetilde{k}) + \varepsilon\,\partial_j B(r)\cdot M(\widetilde{k}) \\ &= -\partial_j\phi(r) + \big(\dot r\times B(r)\big)_j + \varepsilon\,\mathcal{A}_l(\widetilde{k})\,\partial_{r_j} F_{\mathrm{Lor}\,l}(r,\widetilde{k}) + \varepsilon\,\partial_j B(r)\cdot M(\widetilde{k})\,,\end{aligned}$$

as claimed in (60).

Next we substitute (61) and (62). In the following computations we frequently use Taylor expansion to first order and drop terms of order ε^2 without notice. In particular in the terms of order ε one can replace r by q and $\widetilde{k}$ by v. We find that

$$\begin{aligned}\dot q_j &= \dot r_j + \varepsilon\,\dot{\mathcal{A}}_j(v) \\ &= \partial_j E(v) - \varepsilon\,\Big(\mathcal{A}(v)\times B(q)\Big)_l\partial_l\partial_j E(v) \\ &\quad -\varepsilon\,\partial_{v_j}\Big(\big(-\nabla\phi(q) + \nabla E(v)\times B(q)\big)_l\mathcal{A}_l(v) + B(q)\cdot M(v)\Big) \\ &\quad +\varepsilon\partial_l\mathcal{A}_j\dot v_l \\ &= \partial_j E(v) - \varepsilon\dot v_l\Big(\partial_j\mathcal{A}_l - \partial_l\mathcal{A}_j\Big) - \varepsilon\,B(q)\cdot\partial_j M(v) \\ &= \partial_j E(v) - \varepsilon\big(\dot v\times\Omega(v)\big)_j - \varepsilon\,B(q)\cdot\partial_j M(v)\,,\end{aligned}$$

where we used already that $\dot{v} = F_{\mathrm{Lor}} + \mathcal{O}(\varepsilon)$. Thus we obtained the first equation of (4). For the second equation we find

$$\begin{aligned}
\dot{v}_j &= \dot{\tilde{k}}_j + \varepsilon \frac{\mathrm{d}}{\mathrm{d}t}\Big(\mathcal{A}(v) \times B(q)\Big) \\
&= -\partial_j \phi(q) + \varepsilon \mathcal{A}_l(v) \partial_l \partial_j \phi(q) \\
&\quad + \big(\dot{q} \times B(q)\big)_j - \varepsilon\big(\dot{\mathcal{A}}(v) \times B(q)\big)_j - \varepsilon\Big(\dot{q} \times \big(\mathcal{A}_l(v)\partial_l B(q)\big)\Big)_j \\
&\quad + \varepsilon\, \mathcal{A}_l(v) \partial_{q_j} F_{\mathrm{Lor}\, l}(q,v) + \varepsilon\, \partial_j B(q) \cdot M(v) \\
&\quad + \varepsilon\big(\dot{\mathcal{A}}(v) \times B(q)\big)_j + \varepsilon\Big(\mathcal{A}(v) \times \big(\dot{q}_l \partial_l B(q)\big)\Big)_j \\
&= -\partial_j \phi(q) + \big(\dot{q} \times B(q)\big)_j + \varepsilon\, \partial_j B(q) \cdot M(v)\,,
\end{aligned}$$

where the fact that

$$\varepsilon\, \mathcal{A}(v)\Big(\partial_{q_j} F_{\mathrm{Lor}\, l}(q,v) + \partial_l \partial_j \phi(q)\Big) = \varepsilon\, \mathcal{A}_l(v)\Big(\dot{q} \times \partial_j B(q)\Big)_l + \mathcal{O}(\varepsilon^2)$$

cancels the remaining two terms is not so obvious, but can be checked by direct computation. □

A Operator-valued Weyl calculus for τ-equivariant symbols

The quantization of symbols which are functions not on the phase space $\mathbb{R}^{2d}$, but on the cotangent bundle of a more general configuration manifold is a widely studied topic. However, since geometric quantization approaches do not yield a Weyl-Moyal calculus, they are of little use in the adiabatic perturbation theory as developed in [PST_1]. On the other hand, it is rather straightforward to translate the well developed theory for the configuration space $\mathbb{R}^d$ to a flat torus by restricting to periodic functions and symbols. This approach is used by Gérard and Nier [GeNi] in the context of scattering theory in periodic media.

In this appendix we present a similar approach to Weyl quantization of operator-valued symbols which are not exactly periodic, but τ-equivariant with respect to some nontrivial representation τ of the group of lattice translations. We obtain a pseudodifferential and semiclassical calculus which can be applied to τ-equivariant symbols like the Schrödinger Hamiltonian with periodic potential in the Bloch-Floquet representation. In particular, the full computational power of the usual Weyl calculus is retained. The strategy is to use the strong results available for phase space $\mathbb{R}^{2d}$ by restricting to functions which are τ-equivariant in the configurational variable.

Let $\Gamma \subset \mathbb{R}^d$ be a regular lattice generated through the basis $\{\gamma_1, \ldots, \gamma_d\}$, $\gamma_j \in \mathbb{R}^d$, i.e.

$$\Gamma = \Big\{x \in \mathbb{R}^d : x = \textstyle\sum_{j=1}^d \alpha_j\, \gamma_j \ \text{ for some } \alpha \in \mathbb{Z}^d\Big\}\,.$$

Clearly the translations on $\mathbb{R}^d$ by elements of Γ form an abelian group isomorphic to $\mathbb{Z}^d$. The centered fundamental cell of Γ is denoted as

$$B = \Big\{ x \in \mathbb{R}^d : x = \textstyle\sum_{j=1}^d \alpha_j \, \gamma_j \ \text{ for } \alpha_j \in [-\frac{1}{2}, \frac{1}{2}] \Big\} .$$

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

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

If more than one Hilbert space appears, then τ denotes a collection of such representations, i.e. one on each Hilbert space.
Warning: In the application of the results of this appendix to Bloch electrons the lattice Γ corresponds to the dual lattice Γ^* in momentum space $\mathbb{R}^d$, the extended zone scheme.

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

Definition 18. 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 $\big(\tau(\gamma)T\big)(\varphi) = T\big(\tau(\gamma)^{-1} \varphi\big)$ for $\varphi \in \mathcal{S}(\mathbb{R}^d, \mathcal{H})$. The subspace of τ-equivariant distributions is denoted as $\mathcal{S}'_\tau$. Analogously we define

$$\mathcal{H}_\tau = \Big\{ \psi \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathcal{H}) : \ \psi(x - \gamma) = \tau(\gamma) \, \psi(x) \quad \text{for all } \gamma \in \Gamma \Big\} ,$$

which, equipped with the inner product

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

is a Hilbert space. Clearly

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

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

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

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

Now that we have τ-equivariant functions, we define τ-equivariant symbols. To this end we first recall the definition of the standard symbol classes.

Definition 19. A function $w : \mathbb{R}^{2d} \to [0, +\infty)$ is said to be an **order function**, if there exist constants $C_0 > 0$ and $N_0 > 0$ such that

$$w(x) \leq C_0 \, \langle x - y \rangle^{N_0} \, w(y)$$

for every $x, y \in \mathbb{R}^{2d}$. ♢

It is obvious and will be used implicitly that the product of two order functions is again an order function.

Definition 20. A function $A \in C^\infty(\mathbb{R}^{2d}, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ belongs to the symbol class $S^w(\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ with order function w, if for every $\alpha, \beta \in \mathbb{N}^d$ there exists a positive constant $C_{\alpha,\beta}$ such that

$$\left\|(\partial_q^\alpha \partial_p^\beta A)(q,p)\right\|_{\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)} \leq C_{\alpha,\beta}\ w(q,p) \tag{63}$$

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

Definition 21. A map $A : [0, \varepsilon_0) \to S_w(\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)), \varepsilon \mapsto A_\varepsilon$ is a semiclassical symbol of order w, if there exists a sequence $\{A_j\}_{j\in\mathbb{N}} \subset A_j \in S^w(\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ such that

$$A \asymp \sum_{j=0}^{\infty} \varepsilon^j A_j \quad \text{in} \quad S^w(\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))\,,$$

which means that for every $n \in \mathbb{N}$ and for all $\alpha, \beta \in \mathbb{N}^d$ there exists a constant $C_{\alpha,\beta,n}$ such that for any $\varepsilon \in [0, \varepsilon_0)$ one has

$$\left\|\partial_q^\alpha \partial_p^\beta \Big(A_\varepsilon(q,p) - \sum_{j=0}^{n-1} \varepsilon^j A_j(q,p)\Big)\right\|_{\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)} \leq \varepsilon^n\, C_{\alpha,\beta,n}\ w(q,p)\,. \tag{64}$$

The space of semiclassical symbols of order w is denoted as $S^w(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ or, if clear from the context or if no specification is required, as $S^w(\varepsilon)$. The space of formal power series with coefficients in $S^w(\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ is denoted as $M^w(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$.

$\diamondsuit$

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

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

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

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

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

$$K_A(x,y) = \frac{1}{(2\pi\varepsilon)^d} \int_{\mathbb{R}^d} \mathrm{d}\xi\, A\big(\tfrac{1}{2}(x+y), \xi\big)\ \mathrm{e}^{\mathrm{i}\xi\cdot(x-y)/\varepsilon}\,. \tag{65}$$

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

$$K_A(x-\gamma, y-\gamma) = \tau_2(\gamma)\, K_A(x,y)\, \tau_1(\gamma)^{-1} \quad \text{for all } \gamma \in \Gamma\,. \tag{66}$$

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

Proposition 23. *Let $A \in S^w_\tau(\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2))$, then*

$$\widehat{A}\,\mathcal{S}'_{\tau_1}(\mathbb{R}^d,\mathcal{H}_1) \subset \mathcal{S}'_{\tau_2}(\mathbb{R}^d,\mathcal{H}_2)\,.$$

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

To this end notice that as acting on $\mathcal{S}(\mathbb{R}^d,\mathcal{H}_2)$ one finds by direct computation using (65) that $\widehat{A^*}\,L_\gamma = L_\gamma\,(\tau_1(\gamma)^{-1})^*\,\widehat{A^*}\,\tau_2(\gamma)^*$. Indeed, let $\psi \in \mathcal{S}(\mathbb{R}^d,\mathcal{H}_2)$, then

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

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

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

□

For the convenience of the reader we also recall the definition and the basic result about the Weyl product of semiclassical symbols. For a proof see e.g. [DiSj].

Proposition 24. *Let $A \in S^{w_1}(\varepsilon,\mathcal{B}(\mathcal{H}_2,\mathcal{H}_3))$ and $B \in S^{w_2}(\varepsilon,\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2))$, then $\widehat{A}\widehat{B} = \widehat{C}$, with $C \in S^{w_1w_2}(\varepsilon,\mathcal{B}(\mathcal{H}_1,\mathcal{H}_3))$ given through*

$$C(\varepsilon,q,p) = \exp\left(\frac{\mathrm{i}\,\varepsilon}{2}\,(\nabla_p\cdot\nabla_x - \nabla_\xi\cdot\nabla_q)\right)A(\varepsilon,q,p)B(\varepsilon,x,\xi)\Big|_{x=q,\xi=p} =: A\,\widetilde{\sharp}\,B\,. \tag{67}$$

The corresponding product on the level of the formal power series is called Moyal product and denoted as

$$\sharp : M^{w_1}(\varepsilon,\mathcal{B}(\mathcal{H}_2,\mathcal{H}_3)) \times M^{w_2}(\varepsilon,\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)) \to M^{w_1w_2}(\varepsilon,\mathcal{B}(\mathcal{H}_1,\mathcal{H}_3))\,.$$

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

Proposition 25. *Let $A_\varepsilon \in S^{w_1}_\tau(\varepsilon, \mathcal{B}(\mathcal{H}_2, \mathcal{H}_3))$ and $B_\varepsilon \in S^{w_2}_\tau(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$, then $A_\varepsilon B_\varepsilon \in S^{w_1 w_2}_\tau(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_3))$ and $A_\varepsilon \,\widetilde{\sharp}\, B_\varepsilon \in S^{w_1 w_2}_\tau(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_3))$.*

Proof. One has

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

which shows $A_\varepsilon B_\varepsilon \in S^{w_1 w_2}_\tau(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_3))$ and inserted into (67) yields immediately also $A_\varepsilon \,\widetilde{\sharp}\, B_\varepsilon \in S^{w_1 w_2}_\tau(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_3))$. □

An analogous statement holds for the Moyal product of formal symbols.

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

Theorem 26. *Let $A \in S^1_\tau(\mathcal{B}(\mathcal{H}))$ and τ_1, τ_2 unitary representations of Γ in $\mathcal{B}(\mathcal{H})$, then $\widehat{A} \in \mathcal{B}(\mathcal{H}_{\tau_1}, \mathcal{H}_{\tau_2})$ and for $A_\varepsilon \in S^1_\tau(\varepsilon, \mathcal{B}(\mathcal{H}))$ we have that*

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

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

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

Let $j = 1, 2$, then $\mathcal{H}_{\tau_j} \subset L^2_w$ and for any $\psi \in \mathcal{H}_{\tau_j}$ one has the norm equivalence

$$C_1 \|\psi\|_{\mathcal{H}_{\tau_j}} \le \|\psi\|_{L^2_w} \le C_2 \|\psi\|_{\mathcal{H}_{\tau_j}} \tag{68}$$

for appropriate constants $0 < C_1, C_2 < \infty$. The first inequality in (68) is obvious and the second one follows by exploiting τ_j-equivariance of ψ and unitarity of τ_j:

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

According to (68) it suffices to show that $\widehat{A} \in \mathcal{B}(L^2_w)$ and to estimate the norm of $\widehat{A}_\varepsilon$ in this space.

Let $\psi \in C^\infty_{\tau_1}(\mathbb{R}^d, \mathcal{H})$, then by the general theory $\widehat{A}\psi$ is smooth as well (cf. [Fo], Corollary 2.62) and thus, according to Proposition 23, $\widehat{A}\psi \in C^\infty_{\tau_2}(\mathbb{R}^d, \mathcal{H})$. Hence we can use (68) and find

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

However, by Proposition 24, we have that $w\,\widetilde{\sharp}\,A\,\widetilde{\sharp}\,w^{-1} \in S^1(\varepsilon, \mathcal{B}(\mathcal{H}))$. Thus from the usual Calderon-Vaillancourt theorem it follows that

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

This shows that for $A \in S^1_\tau(\mathcal{B}(\mathcal{H}))$ we have $\widehat{A} \in \mathcal{B}(\mathcal{H}_{\tau_1}, \mathcal{H}_{\tau_2})$. Since also $w\,\widetilde{\sharp}\,A_\varepsilon\,\widetilde{\sharp}\,w^{-1} \in S^1(\varepsilon, \mathcal{B}(\mathcal{H}))$ for $A_\varepsilon \in S^1_\tau(\varepsilon, \mathcal{B}(\mathcal{H}))$, we conclude that

$$\sup_{\varepsilon\in[0,\varepsilon_0)} \|\widehat{A}_\varepsilon\|_{\mathcal{B}(\mathcal{H}_{\tau_1}, \mathcal{H}_{\tau_2})} < \infty$$

by the same argument. □

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

$$\sup_{\gamma\in\Gamma} \|\tau_j(\gamma)\|_{\mathcal{B}(\mathcal{H})} \leq C\,, \quad j = 1, 2\,.$$

♢

Finally we would also like to show that for $A \in S^1_\tau(\mathcal{B}(\mathcal{H}))$ the adjoint of $\widehat{A}$ as an operator in $\mathcal{B}(\mathcal{H}_\tau)$, denoted by $\widehat{A}^\dagger$, is given through the quantization of the pointwise adjoint, i.e. through $\widehat{A^*}$. Here it is crucial that τ is a unitary representation.

Proposition 28. *Let $S^1_\tau(\mathcal{B}(\mathcal{H}))$ with a unitary representation τ (with $\tau_1 = \tau_2 = \tau$) and let $\widehat{A}^\dagger$ be the adjoint of $\widehat{A} \in \mathcal{B}(\mathcal{H}_\tau)$, then $\widehat{A}^\dagger = \widehat{A^*}$.*

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

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

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

In particular, we used the τ-equivariance of the kernel (66) and of the functions in $\mathcal{H}_\tau$ and the unitarity of τ. By density we have $\widehat{A^*} = \widehat{A}^\dagger$. □

Acknowledgements. G. P. is grateful for financial support by the Research Training Network HYKE of the European Union and by the Priority Program "Analysis, Modeling and Simulation of Multiscale Problems" of the Deutsche Forschungsgemeinschaft.

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