Effective dynamics for Bloch electrons: Peierls substitution and beyond

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Abstract
We consider an electron moving in a periodic potential and subject to an additional slowly varying external electrostatic potential, \( \phi(\varepsilon x) \), and vector potential \( A(\varepsilon x) \), with \( x \in \mathbb{R}^d \) and \( \varepsilon \ll 1 \). We prove that associated to an isolated family of Bloch bands there exists an almost invariant subspace of \( L^2(\mathbb{R}^d) \) and an effective Hamiltonian governing the evolution inside this subspace to all orders in \( \varepsilon \). To leading order the effective Hamiltonian is given through the Peierls substitution. We explicitly compute the first order correction. From a semiclassical analysis of this effective quantum Hamiltonian we establish the first order correction to the standard semiclassical model of solid state physics.

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1 Introduction

A central problem of solid state physics is to understand the motion of electrons in the periodic potential generated by the ionic cores. While the dynamics 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 $V_\Gamma$ on the electron dynamics consists in changing the dispersion relation from the free kinetic energy $E_{\text{free}}(k) = \frac{1}{2} k^2$ to the modified kinetic energy $E_n(k)$ given by the $n^{\text{th}}$ Bloch band. Otherwise the electron responds to slowly varying external potentials $A, \phi$ as in the case of a vanishing periodic potential. Therefore the semiclassical equations of motion read

$$\dot{r} = \nabla E_n(\kappa), \quad \dot{\kappa} = -\nabla \phi(r) + \dot{r} \times B(r),$$

where $r \in \mathbb{R}^3$ is the position of the electron, $\kappa = k - A(r)$ its kinetic momentum with $k$ its Bloch momentum, $-\nabla \phi$ the external electric field, and $B = \nabla \times A$ the external magnetic field. Note that there is a semiclassical evolution for each Bloch band separately. (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).

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

$$i \varepsilon \partial_t \psi(x,t) = \left( \frac{1}{2} (-i \nabla_x - A(\varepsilon x))^2 + V_\Gamma(x) + \phi(\varepsilon x) \right) \psi(x,t)$$

$$= H^\varepsilon \psi(x,t)$$

in the limit $\varepsilon \to 0$ at leading order. Here the potential $V_\Gamma : \mathbb{R}^3 \to \mathbb{R}$ is periodic with respect to some regular lattice $\Gamma$. $\Gamma$ is generated through the basis $\{\gamma_1, \gamma_2, \gamma_3\}, \gamma_j \in \mathbb{R}^3$, i.e.

$$\Gamma = \left\{ x \in \mathbb{R}^3 : x = \sum_{j=1}^{3} \alpha_j \gamma_j \text{ for some } \alpha \in \mathbb{Z}^3 \right\},$$

and $V_\Gamma(x + \gamma) = V_\Gamma(x)$ for all $\gamma \in \Gamma, x \in \mathbb{R}^3$. The spacing of the lattice $\Gamma$ defines the microscopic spatial scale. The external potentials $A(\varepsilon x)$ and $\phi(\varepsilon x)$, with $A : \mathbb{R}^3 \to \mathbb{R}^3$ and $\phi : \mathbb{R}^3 \to \mathbb{R}$, are slowly varying on the scale of the lattice, as expressed through the dimensionless scale parameter $\varepsilon$, $\varepsilon \ll 1$. 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, see [AsMe], Chapter 12.

In solid state physics the derivation of the semiclassical model (1) received a lot of attention during the 1950s to the 1970s. We mention representatively the work by Luttinger [Lu], Kohn [Ko], Blount [Bl1, Bl2] and Zak [Za]. As late as 1962 Wannier [Wa] argues that the derivation of (1) from (2) is still incomplete.

On the mathematical side the semiclassical asymptotics of the spectrum of $H^\varepsilon$ have been studied in great detail by Gérard, Martinez and Sjöstrand...
GMS with predecessors BeRa Bu HeSj Ne. The large time asymptotics of the solutions to (2) without external potentials is studied in AsKn and the scattering theory is developed in GeNi. However for the dynamics of wave functions, our interest here, the results are modest. In GMMP the case $\phi = 0, A = 0$ is considered, in HST and BMP a proof is given for $A = 0$, which leaves out many interesting applications. The method of Gaussian beams is developed in GRT for a weak uniform magnetic field and in DGR for magnetic Bloch bands.

In fact, as our title indicates, we are more ambitious and plan to derive also the first order correction to (1). The electron acquires then a $k$-dependent electric moment $A_n(k)$ and magnetic moment $M_n(k)$. If the $n$th band is nondegenerate (hence isolated) with Bloch eigenfunctions $\psi_n(k, x)$, the electric dipole moment is given by the Berry connection

$$A_n(k) = i \langle \psi_n(k), \nabla_k \psi_n(k) \rangle$$

and the magnetic moment by the Rammal-Wilkinson term

$$M_n(k) = \frac{1}{2} \langle \nabla_k \psi_n(k), \times (H_{\text{per}}(k) - E(k)) \nabla_k \psi_n(k) \rangle.$$ (4)

Here $\langle \cdot, \cdot \rangle$ denotes the inner product in $L^2(\mathbb{R}^3/\Gamma)$ and $H_{\text{per}}(k)$ is $H^\varepsilon$ of (2) with $\phi = 0 = A$ for fixed Bloch momentum $k$, see Eq. (17). As will be explained in detail, the corrected semiclassical equations read

$$\dot{r} = \nabla_k \left( E_n(k) - \varepsilon B(r) \cdot M_n(k) \right) - \varepsilon \dot{k} \times \Omega_n(k),$$

$$\dot{k} = -\nabla_r \left( \phi(r) - \varepsilon B(r) \cdot M_n(k) \right) + \dot{r} \times B(r)$$

with $\Omega_n(k) = \nabla \times A_n(k)$ the curvature of the Berry connection.

The issue of first order corrections to the semiclassical equations of motion has been investigated recently by Sundaram and Niu SuNi in the context of magnetic Bloch bands, see also Chang and Niu ChNi. One adds in (2) a strong uniform magnetic field $B_0$, i.e. the vector potential $A_0(x) = \frac{1}{2} B_0 \times x$. If its magnetic flux per unit cell is rational, then the Hamiltonian in (2) is still periodic at the expense of a larger unit cell and replacing the usual translations by the magnetic translations. Equation (5) remains formally unaltered, only $E_n$ now refers to the energy of the magnetic subband. Instructive plots of $\Omega_n$ and $M_n$ are provided in SuNi for the particular case of the 2-dimensional Hofstadter model at rational flux $1/3$. The first order corrections obtained in SuNi agree with our equation (5), except for the term of order $\varepsilon$ in the second equation. On a technical level magnetic Bloch bands require some extra considerations and we defer them to a forthcoming paper PST3.

It has been recognized repeatedly, as e.g. emphasized in ABL, that the geometric phases appearing in the first order correction contain novel physics as compared to the leading order. Bloch electrons are no exception. For example for the case of magnetic Bloch bands, the equations of motion (5) provide a
simple semiclassical explanation of the quantum Hall effect. Let us specialize to two dimensions and take $B(r) = 0$, $\phi(r) = -E \cdot r$, i.e. a weak driving electric field and a strong uniform magnetic field with rational flux. Then, since $\kappa = k$, the equations of motion become $\dot{r} = \nabla_k E_n(k) + \mathcal{E}^\perp \Omega_n(k)$, $\dot{k} = \mathcal{E}$, where $\Omega_n$ is now scalar, and $\mathcal{E}^\perp$ is $\mathcal{E}$ rotated by $\pi/2$. We assume initially $k(0) = k$ and a completely filled band, which means to integrate with respect to $k$ over the first Brillouin zone $M^*$. Then the average current for band $n$ is given by

$$j_n = \int_{M^*} dk \dot{r}(k) = \int_{M^*} dk \left( \nabla_k E_n(k) - \mathcal{E}^\perp \Omega_n(k) \right) = -\mathcal{E}^\perp \int_{M^*} dk \Omega_n(k).$$

$\int_{M^*} dk \Omega_n(k)$ is the Chern number of the magnetic Bloch bundle and as such an integer. Further applications related to the semiclassical first order corrections are the anomalous Hall effect [JNM] and the thermodynamics of the Hofstadder model [GaAv].

Our derivation of (5) from (2) proceeds in two conceptually and mathematically distinct steps. The first step is to obtain an effective Hamiltonian whose unitary group closely approximates the solution to the Schrödinger equation (2) for $\varepsilon$ small, in case the initial wave function lies in a subspace corresponding to a prescribed family of Bloch bands. Inside the family, band crossings and almost crossings are allowed. It is crucial however that for every $k$ the family of bands is separated by a gap from the remaining energy bands. Then, associated to the given family of bands, there is a subspace $\Pi^* L^2(\mathbb{R}^3)$ which is adiabatically decoupled from its orthogonal complement to all orders in $\varepsilon$. The effective Hamiltonian generates the approximate time evolution in $\Pi^* L^2(\mathbb{R}^3)$.

Compared to the space-adiabatic perturbation theory developed in [PST1], as a new element we have to face the fact that the classical phase space is $(\mathbb{R}^3/\Gamma^*) \times \mathbb{R}^3$, $\Gamma^*$ the lattice dual to $\Gamma$ and $\mathbb{R}^3/\Gamma^* = M^*$ the first Brillouin zone. To come close to the scheme in [PST1] a natural approach is to use the extended zone scheme. Going from one cell to the next, one picks up a phase factor which necessitates to generalize the pseudodifferential calculus to $\tau$-equivariant symbols, see Appendix A.

The effective Hamiltonian is expanded in an $\varepsilon$-independent reference Hilbert space. For example, for a nondegenerate band the reference space is $L^2(M^*, dk)$ and the leading order effective Hamiltonian is given through the Peierls substitution

$$h_0(k, i\varepsilon \nabla_k) = E_n(k - A(i\varepsilon \nabla_k)) + \phi(i\varepsilon \nabla_k),$$

where $i\nabla_k$ is understood with periodic boundary conditions on $M^*$.

The natural second step consists in a semiclassical analysis of the effective Hamiltonian. It is a standard result that the unitary group generated by $h_0$ is well approximated by the semiclassical equations (1). At next order, $h_0(k, i\varepsilon \nabla_k)$ is corrected to $h_0(k, i\varepsilon \nabla_k) + \varepsilon h_1(k, i\varepsilon \nabla_k)$, with $h_1$ given in (22). However (5) is not the semiclassical evolution corresponding to that Hamiltonian. The reason is that the subspace $\Pi^* L^2(\mathbb{R}^3)$ is mapped to the reference Hilbert space $L^2(M^*, dk)$ through a unitary operator which itself depends on $\varepsilon$. Therefore,
the transformation of observables generates an $\varepsilon$-dependence in addition to the transformation of time-evolved states. If done properly, one arrives at (5).

To give a brief outline of the paper. In Section 2 we discuss the periodic Hamiltonian. In particular we recall the unitary Zak transform and state our assumptions on $V_\Gamma$, $A$, $\phi$ and the gap condition. In Section 3 we apply the space-adiabatic perturbation theory to the present case, using the pseudodifferential calculus developed in Appendix A. The semiclassical analysis of the effective Hamiltonian including first order is carried out in Section 4. The precise link between (2) and (5) is stated in Theorem 11. In Appendix B we show that the equations (5) are of Hamiltonian form with respect to an appropriate symplectic structure.

2 The periodic Hamiltonian

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

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

acting in $L^2(\mathbb{R}^d)$, keeping from now on the dimension $d$ arbitrary. The potential $V_\Gamma$ is periodic with respect to the lattice $\Gamma$. Its dual lattice $\Gamma^*$ is defined as the lattice generated by the dual basis $\{\gamma^*_1, \ldots, \gamma^*_d\}$ determined through the conditions $\gamma_i \cdot \gamma^*_j = 2\pi \delta_{ij}$, $i,j \in \{1, \ldots, d\}$. The centered fundamental domain of $\Gamma$ is denoted by $M = \{x \in \mathbb{R}^d : x = \sum_{j=1}^d \alpha_j \gamma_j \text{ for } \alpha_j \in [-\frac{1}{2}, \frac{1}{2}]\}$, and analogously the centered fundamental domain of $\Gamma^*$ is denoted by $M^*$. In solid state physics the set $M^*$ is called the first Brillouin zone. In the following $M^*$ is always equipped with the normalized Lebesgue measure denoted by $dk$.

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 $k = |k| + \gamma^*$.

We employ a variant of the Bloch-Floquet transform, called the Zak transform (also Lifshitz-Gelfand-Zak transform). The Zak transform of a function $\psi \in S(\mathbb{R}^d)$ is defined as

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

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

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

$$\langle \mathcal{U}\psi \rangle(k + \gamma^*, y) = e^{-iy \cdot \gamma^*} \langle \mathcal{U}\psi \rangle(k, y) \quad \text{for all } \gamma^* \in \Gamma^*.$$
From [5] it follows that, for any fixed \( k \in \mathbb{R}^d \), \((U\psi)(k,\cdot)\) is a \( \Gamma \)-periodic function and can thus 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 translations on \( \Gamma^* \) (denoted again as \( \Gamma^* \) with a little abuse of notation), given by

\[
\tau : \Gamma^* \to \mathcal{U}(L^2(\mathbb{T}^d)), \quad \gamma^* \mapsto \tau(\gamma^*), \quad (\tau(\gamma^*)\varphi)(y) = e^{i\gamma^* \cdot \varphi(y)}.
\]

It will turn out convenient to introduce the Hilbert space

\[
\mathcal{H}_\tau := \left\{ \psi \in L^2_{\text{loc}}(\mathbb{R}^d, L^2(\mathbb{T}^d)) : \psi(k - \gamma^*) = \tau(\gamma^*) \psi(k) \right\}, \tag{10}
\]

equipped with the inner product

\[
\langle \psi, \varphi \rangle_{\mathcal{H}_\tau} = \int_{\mathbb{R}^d} dk \langle \psi(k), \varphi(k) \rangle_{L^2(\mathbb{T}^d)}.
\]

Notice that if one considers the trivial representation, i.e. \( \tau \equiv 1 \), then \( \mathcal{H}_\tau \) is simply a space of \( \Gamma^* \)-periodic vector-valued functions over \( \mathbb{R}^d \).

Obviously, there is a natural isomorphism between \( \mathcal{H}_\tau \) and \( L^2(M^*, L^2(\mathbb{T}^d)) \) given by restriction from \( \mathbb{R}^d \) to \( M^* \), and with inverse given by \( \tau \)-equivariant continuation, as suggested by [4]. The reason for working with \( \mathcal{H}_\tau \) instead of \( L^2(M^*, L^2(\mathbb{T}^d)) \) is twofold. First of all it allows to apply the pseudodifferential calculus as developed in Appendix A. 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

\[
\mathcal{U} : L^2(\mathbb{R}^d) \to \mathcal{H}_\tau \cong L^2(M^*, L^2(\mathbb{T}^d)) \cong L^2(M^*) \otimes L^2(\mathbb{T}^d).
\]

\( \mathcal{U} \) is an isometry and \( \mathcal{U}^{-1} \) given through

\[
(\mathcal{U}^{-1} \varphi)(x) = \int_{M^*} dk \ e^{i\gamma^* \cdot k} \varphi(k, [x]) \tag{11}
\]

satisfies \( \mathcal{U}^{-1} \mathcal{U} \psi = \psi \) for \( \psi \in \mathcal{S}(\mathbb{R}^d) \), as can be checked by direct calculation. \( \mathcal{U}^{-1} \) 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, thus unitary.

In order to determine the Zak transform of operators like the full Hamiltonian in [2], we need to discuss how differential and multiplication operators behave under the Zak transform, see [Bl1], [Za]. Let \( P = -i\nabla_x \) with domain \( H^1(\mathbb{R}^d) \) and \( Q \) multiplication by \( x \) on the maximal domain. Then

\[
\mathcal{U} P \mathcal{U}^{-1} = 1 \otimes -i \nabla^\text{per}_y + k \otimes 1, \tag{12}
\]

\[
\mathcal{U} Q \mathcal{U}^{-1} = i \nabla_k^L, \tag{13}
\]

where \(-i \nabla^\text{per}_y\) is equipped with periodic boundary conditions or, equivalently, operating on the domain \( H^1(\mathbb{T}^d) \). The domain of \( i \nabla_k^L \) is \( \mathcal{H}_\tau \cap H^1_{\text{loc}}(\mathbb{R}^d, L^2(\mathbb{T}^d)) \), i.e. it consists of distributions in \( H^1(M^*, L^2(\mathbb{T}^d)) \) which satisfy the \( y \)-dependent boundary condition associated with [3]. In addition to (12) and (13) we notice
that multiplication with a $\Gamma$-periodic function like $V_{\Gamma}$ is mapped into multiplication with the same function, i.e. $\mathcal{U} V_{\Gamma}(x) \mathcal{U}^{-1} = 1 \otimes V_{\Gamma}(y)$.

For later use we remark that the following relations can be checked using the definitions \ref{7} and \ref{11},
\[
\psi \in H^m(\mathbb{R}^d), \ m \geq 0 \iff \mathcal{U}\psi \in L^2(B, H^m(\mathbb{T}^d)),
\]
\[
\langle x \rangle^m \psi(x) \in L^2(\mathbb{R}^d), \ m \geq 0 \iff \mathcal{U}\psi \in \mathcal{H}_r \cap \mathcal{H}_{\text{loc}}^m(\mathbb{R}^d, L^2(\mathbb{T}^d)).
\]

**Remark 1.** The Bloch-Floquet transform is usually defined as
\[
(\tilde{\mathcal{U}}\psi)(k, x) := \sum_{\gamma \in \Gamma} e^{-i\gamma \cdot k} \psi(x + \gamma), \ (k, x) \in \mathbb{R}^{2d}.
\]
for $\psi \in \mathcal{S}(\mathbb{R}^d)$. In contrast to \ref{14}, functions in the range of $\tilde{\mathcal{U}}$ are periodic in $k$ and quasi-periodic in $y$,
\[
(\tilde{\mathcal{U}}\psi)(k, y + \gamma) = e^{i\gamma \cdot k} (\tilde{\mathcal{U}}\psi)(k, y) \quad \text{for all} \quad \gamma \in \Gamma,
\]
\[
(\tilde{\mathcal{U}}\psi)(k + \gamma^* , y) = (\tilde{\mathcal{U}}\psi)(k, y) \quad \text{for all} \quad \gamma^* \in \Gamma^*.
\]
Our choice of using the Zak transform $\mathcal{U}$ instead of $\tilde{\mathcal{U}}$ comes from the fact that the transform of the gradient has a domain which is independent of $k \in M^*$, see \ref{15}. As we shall see, this is essential for the application of the pseudodifferential calculus of Appendix A.

For the Zak transform of the free Hamiltonian one finds
\[
\mathcal{U} H_{\text{per}} \mathcal{U}^{-1} = \int_{M^*} dk H_{\text{per}}(k)
\]
with
\[
H_{\text{per}}(k) = \frac{1}{2} \left( -i \nabla_y + k \right)^2 + V_{\Gamma}(y), \quad k \in M^*.
\]
For fixed $k \in M^*$ the operator $H_{\text{per}}(k)$ acts on $L^2(\mathbb{T}^d)$ with domain $H^2(\mathbb{T}^d)$ independent of $k \in M^*$, whenever the following assumption on the potential is satisfied.

**Assumption A\textsubscript{1}.** We assume that $V_{\Gamma}$ is infinitesimally bounded with respect to $-\Delta$ and that $\phi \in C_b^\infty(\mathbb{R}^d, \mathbb{R})$ and $A_j \in C_b^\infty(\mathbb{R}^d, \mathbb{R})$ for any $j \in \{1, \ldots, d\}$.

Here $C^\infty_b(\mathbb{R}^d, \mathbb{R})$ denotes the space of bounded smooth functions with derivatives of any order bounded. From this assumption it follows in particular that also the full Hamiltonian $H^\varepsilon$ of \ref{2} is self-adjoint on $H^2(\mathbb{R}^d)$. Assumption (A\textsubscript{1}) excludes the case of globally constant electric and magnetic field. However, since we are not concerned with the spectral analysis of $H^\varepsilon$, but with the dynamics of states for large but finite times, locally constant fields serve us as well.

The band structure of the fibered spectrum of $H_{\text{per}}$ is crucial for the following. The resolvent $R^0_\lambda = (H_0(k) - \lambda)^{-1}$ of the operator $H_0(k) = \frac{1}{2} \left( -i \nabla_y + k \right)^2$
is compact for fixed $k \in M^*$. Since, by assumption, $R_{\lambda} V_{T}$ is bounded, also $R_{\lambda} = (H_{\text{per}}(k) - \lambda)^{-1} = R_{\lambda}^0 + R_{\lambda} V_{T} R_{\lambda}^0$ is compact. As a consequence $H_{\text{per}}(k)$ has purely discrete spectrum with eigenvalues of finite multiplicity which accumulate at infinity. A more detailed discussion can be found e.g. in [W1]. For definiteness the eigenvalues are enumerated increasingly as $E_1(k) \leq E_2(k) \leq E_3(k) \leq \ldots$ and repeated according to their multiplicity. The corresponding normalized eigenfunctions $\{\varphi_n(k)\}_{n \in \mathbb{N}} \subset H^2(\mathbb{T}^d)$ are called Bloch functions and form, for any fixed $k$, an orthonormal basis of $L^2(\mathbb{T}^d)$. We will call $E_n(k)$ the $n^{\text{th}}$ band function or just the $n^{\text{th}}$ band. 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

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

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

**Definition 2.** A family of Bloch bands $\{E_n(k)\}_{n \in I}$, $I = [I_-, I_+] \cap \mathbb{N}$, is called isolated, or satisfies the gap condition, if

$$\inf_{k \in M^*} \text{dist} \left( \bigcup_{n \in I} \{E_n(k)\}, \bigcup_{m \notin I} \{E_m(k)\} \right) =: C_\gamma > 0.$$

In the following we fix an index set $I \subset \mathbb{N}$ for an isolated family of bands. Let $P_{\mathcal{I}}(k)$ be the spectral projector of $H_{\text{per}}(k)$ corresponding to the eigenvalues $\{E_n(k)\}_{n \in I}$, then $P_{\mathcal{I}} := \int_{M^*} dk P_{\mathcal{I}}(k)$ defines the projector on the given isolated family of bands. In terms of Bloch functions $P_{\mathcal{I}}(k) = \sum_{n \in I} \langle \varphi_n(k) \rangle \langle \varphi_n(k) \rangle$. 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 [L3] 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 A2.** If the isolated family of bands $\{E_n(k)\}_{n \in I}$ is degenerate, in the sense that $\ell = |I| > 1$, then we assume that there exists an orthonormal basis $\{\psi_j(k)\}_{j=1}^\ell$ of $\text{Ran} P_{\mathcal{I}}(k)$ whose elements are smooth and $\tau$-equivariant with respect to $k$, i.e. $\psi_j(k - \gamma^*) = \tau(\gamma^*) \psi_j(k)$ for all $j \in \{1, \ldots, \ell\}$ and $\gamma^* \in \Gamma^*$.

In the case of a single isolated $\ell$-fold degenerate Bloch band (i.e. $E_n(k) = E_\mu(k)$ for every $n \in \mathcal{I}$, $|\mathcal{I}| = \ell$), Assumption (A2) is equivalent to the existence of an orthonormal basis consisting of smooth and $\tau$-equivariant Bloch functions. On the other side, if there are eigenvalue crossings inside the family of bands, Assumption (A2) requires only that $\psi_j(k)$ is an eigenfunction of the corresponding eigenprojection $P_{\mathcal{I}}(k)$ and not of the free Hamiltonian $H_{\text{per}}(k)$.

From the geometrical viewpoint Assumption (A2) is equivalent to the triviality of a complex vector bundle over $\mathbb{T}^d$, namely the bundle of the null spaces
of $1 - P_\mathcal{T}(k)$ for $k \in M^*$. In this geometrical perspective it is not difficult to see that Assumption (A2) is always satisfied if either $d = 1$ or $\ell = 1$. Indeed, classification theory for bundles implies that any complex vector bundle over $T^1 = S^1$ is trivial. As for $\ell = 1$, it is a classical result, due to Kostant and Weil, that smooth complex line bundles are completely classified by their first integer Chern class. In our case, the time-reversal symmetry of $H_{\text{per}}$ implies the vanishing of the first integer Chern class, and therefore the triviality of the bundle. The same, and indeed slightly stronger, results can be proved with analytical techniques, as in Ne and references therein. By pushing forward the geometrical approach above, we expect that Assumption (A2) is generically satisfied for $d \leq 3$, as it will be discussed in Pa.

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 (A2) fails. As well understood and discussed in the introduction, 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 PST3.

### 3 Space-adiabatic perturbation for Bloch bands

Let $P_n(k) = |\varphi_n(k)\rangle\langle\varphi_n(k)|$. Then the projector on the $n$th band subspace is given through $P_n = \int_M \, dk \, P_n(k)$. By construction the band subspaces are invariant under the dynamics generated by $H_{\text{per}},$

$$\left[ e^{-iH_{\text{per}}t}, P_n \right] = \left[ e^{-iE_n(k)t}, P_n \right] = 0 \quad \text{for all } n \in \mathbb{N}, \ s \in \mathbb{R}.$$  

Notice that $P_n$ is not a spectral projector of $H_{\text{per}},$ in general, since in more than one space dimension it can happen that e.g. $E_n(k) < E_{n+1}(k)$ for all $k \in M^*$ but $\inf_k E_{n+1}(k) < \sup_k E_n(k)$. According to the identity (12), in the original representation $H_{\text{per}}$ acts on the $n$th band subspace as

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

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 $E_n(k)$.

In the presence of non-periodic external fields the subspaces $P_n \mathcal{H}_\tau$ 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 almost invariant subspaces associated with isolated Bloch bands. To construct them, and to study the dynamics inside these almost invariant subspaces, we apply adiabatic perturbation to perturbed Bloch bands.
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 space the action of the full Hamiltonian is given through a semiclassical pseudodifferential operator, whose power series expansion can be computed to any order in \( \varepsilon \). This effective Hamiltonian is constructed in Section 3.3 and we compute explicitly its principal and subprincipal symbol. 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 \( M^* \), or, equivalently, acting on the space \( \mathcal{H}_\tau \). This task is deferred to Appendix A.

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 \( \mathcal{H}_f \) and any unitary representation \( \tau : \Gamma^* \rightarrow \mathcal{U}(\mathcal{H}_f) \), one defines the Hilbert space

\[
L^2_\tau(\mathbb{R}^d, \mathcal{H}_f) := \left\{ \psi \in L^2_{\text{loc}}(\mathbb{R}^d, \mathcal{H}_f) : \psi(k - \gamma^*) = \tau(\gamma^*) \psi(k) \right\},
\]
equipped with the inner product

\[
\langle \psi, \varphi \rangle_{L^2_\tau} = \int_{M^*} dk \langle \psi(k), \varphi(k) \rangle_{\mathcal{H}_f}.
\]

Using the results of the previous section and imposing Assumption (A1), the Zak transform of the full Hamiltonian in (2) is given through

\[
H^\varepsilon_Z := U H^\varepsilon U^{-1} = \frac{1}{2} \left( -i \nabla_y + k - A(i \varepsilon \nabla_k) \right)^2 + V(y) + \phi(i \varepsilon \nabla_k)
\]
with domain \( L^2_\varepsilon(\mathbb{R}^d, H^2(T^d)) \).

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

**Theorem 3 (Peierls substitution and higher order corrections).** Let \( \{E_n\}_{n \in \mathbb{I}} \) be an isolated family of bands, see Definition 2 and let the Assumptions (A1) and (A2) be satisfied. Then there exist

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

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

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

such that

\[
\left\| [H^\varepsilon_Z, \Pi^\varepsilon] \right\| = O(\varepsilon^\infty), \quad \| \Pi^\varepsilon - P_T \| = O(\varepsilon)
\]

10
and
\[ \| (e^{-iHt} - U^\ast e^{-\hat{\mathcal{H}}t} U^\ast) \| = O(\varepsilon^\infty(1 + |t|)). \]

The effective Hamiltonian \( \hat{\mathcal{H}} \) is the Weyl quantization of a semiclassical symbol \( h \in S^2_{\varepsilon \equiv 1}(\varepsilon, \mathcal{B}(\mathbb{C}^d)) \) with an asymptotic expansion to any order. The \( \mathcal{B}(\mathbb{C}^d) \)-valued principal symbol \( h_0(k, r) \) has matrix-elements
\[ h_0(k, r)_{\alpha\beta} = \langle \psi_\alpha(k - A(r)), H_0(k, r) \psi_\beta(k - A(r)) \rangle, \quad (20) \]
where \( \alpha, \beta \in \{1, \ldots, \ell\} \) and \( H_0(k, r) \) is defined in \( \mathbb{P} \).

The general formula for the subprincipal symbol of the effective Hamiltonian can be found in \( \mathbb{PST} \). The structure and the interpretation of the effective Hamiltonian are most transparent for the case of a single isolated band.

**Corollary 4.** For an isolated \( \ell \)-fold degenerate eigenvalue \( E(k) \) the \( \mathcal{B}(\mathbb{C}^d) \)-valued symbol \( h(k, r) = h_0(k, r) + \varepsilon h_1(k, r) + O(\varepsilon^2) \) constructed in Theorem \( \mathbb{P} \) has matrix-elements
\[ h_0(k, r)_{\alpha\beta} = (E(k - A(r)) + \phi(r)) \delta_{\alpha\beta} \quad (21) \]
and
\[ h_1(k, r)_{\alpha\beta} = -\left( -\nabla \phi(r) + \nabla E(\bar{k}) \times B(r) \right) \cdot \mathcal{A}(\bar{k})_{\alpha\beta} - B(r) \cdot \mathcal{M}(\bar{k})_{\alpha\beta} \quad (22) \]
where \( \mathcal{A}(k)_{\alpha\beta} = i \langle \psi_\alpha(k), \nabla \psi_\beta(k) \rangle_{\mathcal{H}_k} \).

In dimension \( d = 3 \) the subprincipal symbol \( 22 \) has a straightforward physical interpretation. The 2-forms \( B \) and \( \mathcal{M} \) are naturally identified with the vectors \( B = \text{curl} A \) and
\[ \mathcal{M}(k)_{\alpha\beta} = \frac{i}{2} \langle \nabla \psi_\alpha(k), \times (H_{\text{per}}(k) - E(k)) \nabla \psi_\beta(k) \rangle_{\mathcal{H}_k}. \]
Therefore the symbol of the effective Hamiltonian has the same form as the energy of a classical charge distribution in weak external fields, in first order multipole expansion. In this sense \( \mathcal{A}(k) \) is interpreted as an effective electric dipole moment and \( \mathcal{M}(k) \) as an effective magnetic dipole moment.

**Remark 5.** 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 \(B, \Omega_n\) and \(M_n\) are 2-forms. The inner product of 2-forms is

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

where \(\ast\) denotes the Hodge duality induced by the euclidian metric, and for a vector field \(w\) and a 2-form \(F\) the “vector product” is

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

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

Theorem 3 is a direct consequence of the results proved in Propositions 6, 8 and 9. The proof of Corollary 4 is given at the end of this section.

As mentioned before, the main idea of the proof is to adapt the general scheme of space-adiabatic perturbation theory to the case of the Bloch electron. While formally this seems straightforward, one must overcome two mathematical problems. First of all, in the present case the symbols are unbounded operator-valued functions. One can deal with unbounded-operator-valued symbols by considering them as bounded operators from their domain equipped with the graph norm into the Hilbert space, see e.g. [DiSj]. The second, more serious problem consists in setting up a Weyl calculus for operators acting on spaces like \(L^2_\tau(\mathbb{R}^d, \mathcal{H}_f)\). This is done in Appendix A and we will use in this section the terminology and notations introduced there.

The results of Appendix A allow us to write the Hamiltonian \(H_0\) as the Weyl quantization \(\hat{H}_0\) of the \(\tau\)-equivariant symbol

\[
H_0(k, r) = \frac{1}{2} \left( -i \nabla_y + k - A(r) \right)^2 + V_\Gamma(x) + \phi(r)
\]

acting on the Hilbert space \(\mathcal{H}_f := L^2(\mathbb{T}^d, dx)\) 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 \(\mathcal{H}_f\) which is \(\tau\)-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 \(\mathcal{H}_f\), see Definition 21. Then the general theory developed in Appendix A can be applied. The usual Weyl quantization of \(H_0\) is an operator from \(S'(\mathbb{R}^d, \mathcal{D})\) to \(S'(\mathbb{R}^d, \mathcal{H}_f)\) given by

\[
\hat{H}_0 = \frac{1}{2} \left( -i \nabla_y + k - A(\imath \nabla_k) \right)^2 + V_\Gamma(y) + \phi(\imath \nabla_k).
\]

Then \(\hat{H}_0\) can be restricted to \(L^2_{loc}(\mathbb{R}^d, \mathcal{D})\), since \(A\) and \(\phi\) are smooth and bounded. Since \(H_0\) is a \(\tau\)-equivariant symbol, \(\hat{H}_0\) preserves \(\tau\)-equivariance and can then be restricted to an operator from \(L^2_\tau(\mathbb{R}^d, \mathcal{D})\) to \(L^2_\tau(\mathbb{R}^d, \mathcal{H}_f)\). To conclude that \(\hat{H}_0\), restricted to \(L^2_\tau(\mathbb{R}^d, \mathcal{D})\), agrees with \(\hat{H}_0\), it is enough to recall that \(i \nabla_k\) is defined as \(i \nabla_k\) restricted to \(H^1 \cap \mathcal{H}_\tau\) and to use the spectral calculus.
Moreover, if one introduces the order function \(w(k, r) := (1 + k^2)\), then \(H_0 \in S^w(B(D, \mathcal{H}))\). More generally, we will give the proofs for any symbol \(H \in S^w(\varepsilon, B(D, \mathcal{H}))\), whose principal symbol is then denoted by \(H_0\).

### 3.1 The almost invariant subspace

In this section we construct the adiabatically decoupled subspace associated with an isolated Bloch band. Similar constructions have a considerable history and we refer to [MaSo, NeSo, PST1, Te1] and references therein.

Given an isolated family of bands \(\{E_n(k)\}_{n \in \mathbb{I}}\), we define \(\pi_0(k, r) = P_I(k - A(r))\). It follows from the \(\tau\)-equivariance of \(H_0\) and from the gap condition that \(\pi_0 \in S^1_{\tau}(B(\mathcal{H}))\). We also define the shorthand \(A(\varepsilon) = O_0(\varepsilon^n)\), where the subscript expresses that a family \(A(\varepsilon) \in B(\mathcal{H})\) is \(O(\varepsilon^n)\) in the norm of bounded operators. By \(A(\varepsilon) = O_0(\varepsilon^\infty)\) we mean that \(A(\varepsilon) = O_0(\varepsilon^n)\) for any \(n \in \mathbb{N}\). The remaining notation is defined in Appendix A.

**Proposition 6.** Let \(\{E_n\}_{n \in \mathbb{I}}\) be an isolated family of bands and let Assumption (A1) be satisfied. Then there exists an orthogonal projection \(\Pi^\varepsilon \in B(\mathcal{H}_\tau)\) such that

\[
[H^\varepsilon, \Pi^\varepsilon] = O_0(\varepsilon^\infty)
\]

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

\[
\pi \simeq \sum_{j \geq 0} \varepsilon^j \pi_j \quad \text{in} \quad S^1_{\tau}(\varepsilon, B(\mathcal{H}))
\]

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

**Proof.** We first construct \(\pi\) on a formal symbol level.

**Lemma 7.** Let \(w(k, r) = (1 + k^2)\). There exists a unique formal symbol

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

such that \(\pi_0(k, r) = P_I(k - A(r))\) and

(i) \(\pi^* \pi = \pi\),

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

(iii) \(H^\pi - \pi^\sharp H = 0\).

**Proof.** We construct the formal symbol \(\pi\) locally in phase space and obtain by uniqueness, which can be proved as in [PST1], 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 \(U_{z_0}\) of \(z_0\)
such that for every $z \in U_{z_0}$ the set $\{E_n(z)\}_{n \in I}$ 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,

$$\text{dist}(\Lambda(z_0), \sigma(H(z))) \geq \frac{1}{4} C_g \quad \text{for all} \quad z \in U_{z_0}$$

(27)

and

$$\text{Radius}(\Lambda(z_0)) \leq C_r.$$  

(28)

The constant $C_g$ appearing in (27) is the same as in Definition 2 and the existence of a constant $C_r$ independent of $z_0$ such that (28) is satisfied follows from the periodicity of $\{E_n(z)\}_{n \in I}$ and the fact that $A$ and $\phi$ are bounded. Indeed, $\Lambda$ can be chosen $\Gamma^*$-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 $z \in U_{z_0}$. We will construct a formal symbol $R(\zeta)$ with values in $B(H_f, D)$ — the local Moyal resolvent of $H$ — such that

$$(H - \zeta) \not\sharp R(\zeta) = 1_{H_f} \quad \text{and} \quad R(\zeta) \not\sharp (H - \zeta) = 1_D \quad \text{on} \quad U_{z_0}.$$  

(29)

To this end let

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

where according to (27) $R_0(\zeta)(z) \in B(H_f, D)$ for all $z \in U_{z_0}$, and, using differentiability of $H(z), \partial^\alpha_z R_0(\zeta)(z) \in B(H_f, D)$ for all $z \in U_{z_0}$. By construction one has

$$(H - \zeta) \not\sharp R_0(\zeta) = 1_{H_f} + O_0(\varepsilon),$$

where the remainder is $O(\varepsilon)$ in the $B(H_f)$-norm. We proceed by induction. Suppose that

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

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

$$(H - \zeta) \not\sharp R^{(n)}(\zeta) = 1_{H_f} + \varepsilon^{n+1} E_{n+1}(\zeta) + O_0(\varepsilon^{n+2}),$$

(30)

where $E_{n+1}(\zeta)(z) \in B(H_f)$. By choosing

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

(31)

we obtain that $R^{(n+1)}(\zeta) = R^{(n)}(\zeta) + \varepsilon^{n+1} R_{n+1}(\zeta)$ takes values in $B(H_f, D)$ and satisfies the first equality in (29) up to $O(\varepsilon^{n+2})$. 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
\( \tilde{R}(\zeta) \) with values in \( B(\mathcal{H}_t, \mathcal{D}) \) which exactly satisfies the second equality in (29). By the associativity of the Moyal product, they must agree:

\[
\tilde{R}(\zeta) = \tilde{R}(\zeta) \ast (H - \zeta) \ast R(\zeta) = R(\zeta) \quad \text{on } \mathcal{U}_{z_0}.
\]

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

\[
R(\zeta) - R(\zeta') = (\zeta - \zeta') R(\zeta) \ast R(\zeta') \quad \text{on } \mathcal{U}_{z_0}
\]

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

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

satisfies (i) and (ii) of Lemma 7. As for (iii) a little bit of care is required. Let \( J : \mathcal{D} \rightarrow \mathcal{H}_t \) be the continuous injection of \( \mathcal{D} \) into \( \mathcal{H}_t \). Using (33) and (32) it follows that \( \pi J \ast R(\zeta) = R(\zeta) J \ast \pi \) for all \( \zeta \in \Lambda(z_0) \). Moyal-multiplying from left and from the right with \( H - \zeta \) one finds \( H \ast \pi J = J \ast \pi H \) as operators in \( B(\mathcal{D}, \mathcal{H}_t) \). However, by construction \( H \ast \pi \) takes values in \( B(\mathcal{H}_t) \) and, by density of \( \mathcal{D} \), the same must be true for \( \pi H \).

We are left to show that \( \pi \in M^1_\varepsilon(\mathcal{H}, B(\mathcal{H}_t)) \cap M^\omega_\varepsilon(\mathcal{H}, B(\mathcal{H}_t, \mathcal{D})) \). To this end notice that by construction \( \pi \) inherits the \( \tau \)-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

\[
\| (\partial^\alpha \pi_j)(z) \| \leq 2\pi C_\tau \sup_{\zeta \in \Lambda(z_0)} \| (\partial^\alpha R_j)(\zeta, z) \|,
\]

where \( \| \cdot \| \) stands either for the norm of \( B(\mathcal{H}_t) \) or for the norm of \( B(\mathcal{H}_t, \mathcal{D}) \). In order to show that \( \pi \in M^1_\varepsilon(\mathcal{H}, B(\mathcal{H}_t)) \) it suffices to consider \( z = (k, r) \in M^* \times \mathbb{R}^d \) since \( \tau(\gamma^*) \) is unitary and thus the \( B(\mathcal{H}_t) \)-norm of \( \pi \) is periodic. According to (32) we must show that

\[
\| (\partial^\alpha R_j)(\zeta, z) \|_{B(\mathcal{H}_t)} \leq C_{\alpha j} \quad \forall z \in \mathcal{U}_{z_0}, \ z \in \Lambda(z_0)
\]

with \( C_{\alpha j} \) independent of \( z_0 \in M^* \times \mathbb{R}^d \).

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

\[
R_j(\zeta) \in S_{1^\varepsilon}(B(\mathcal{H}_t)) \cap S_{1^\tau}(B(\mathcal{H}_t, \mathcal{D}))
\]

uniformly in \( \zeta \), in the sense that the Fréchet semi-norms are bounded by \( \zeta \)-independent constants. Then, according to Proposition (24) \( E_{n+1}(\zeta) \), as defined by (30), belongs to \( S_{1^\varepsilon}(B(\mathcal{H}_t)) \) uniformly in \( \zeta \). By \( \tau \)-equivariance, the norm of \( E_{n+1}(\zeta) \) is periodic and one concludes that \( E_{n+1}(\zeta) \in S_{1^\varepsilon}(B(\mathcal{H}_t)) \) uniformly in \( \zeta \). 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 (37) one has for all \( z \in \mathbb{R}^{2d} \)
\[
\| R_0(\zeta) \|_{\mathcal{B}(\mathcal{H}_t)} = \|(H(z) - \zeta)^{-1}\|_{\mathcal{B}(\mathcal{H}_t)} = \frac{1}{\text{dist}(\zeta, \sigma(H(z)))} \leq \frac{4}{C_\varepsilon}.
\]
By the chain rule,
\[
(\partial_z R_0)(\zeta, z) \|_{\mathcal{B}(\mathcal{H}_t)} = \|(R_0(\zeta)(\partial_z H_0)R_0(\zeta))(z)\|_{\mathcal{B}(\mathcal{H}_t)}. \tag{37}
\]
Since \( \partial_z H_0 R_0(\zeta) \) is a \( \tau \)-equivariant \( \mathcal{B}(\mathcal{H}_t) \)-valued symbol, its norm is periodic. Therefore it suffices to estimate its norm for \( z \in M^* \times \mathbb{R}^d \), which yields the required bound. For a general \( \alpha \in \mathbb{N}^{2d} \), the norm of \( \partial_\alpha^\gamma R_0(\zeta) \) can be bounded in a similar way. This proves that \( R_0(\zeta) \) belongs to \( S^1_{\tau}(\mathcal{B}(\mathcal{H}_t)) \) uniformly in \( \zeta \).

On the other hand
\[
\| R_0(k, r) \|_{\mathcal{B}(\mathcal{H}_t, \mathcal{D})} = \|(1 + \Delta_x) R_0([k] + \gamma^*, r)\|_{\mathcal{B}(\mathcal{H}_t)}
\]
\[
= \|(1 + \Delta_x) \tau(\gamma^*) R_0([k], r) \tau^{-1}(\gamma^*)\|_{\mathcal{B}(\mathcal{H}_t)}
\]
\[
\leq C \|(1 + \gamma^*^2)(1 + \Delta_x) R_0([k], r)\|_{\mathcal{B}(\mathcal{H}_t)}
\]
\[
\leq C'(1 + \gamma^*^2) \leq 2C'(1 + k^2),
\]
where we used the fact that \( \|(1 + \Delta_x) R_0(z)\|_{\mathcal{B}(\mathcal{H}_t)} \) is bounded for \( z \in M^* \times \mathbb{R}^d \).

The previous estimate and the fact that \( \partial_z H_0 R_0(\zeta) \in S^1_{\tau}(\mathcal{B}(\mathcal{H}_t)) \) yield
\[
(\partial_z R_0)(\zeta, z) \|_{\mathcal{B}(\mathcal{H}_t, \mathcal{D})} = \|(R_0(\zeta)(\partial_z H_0)R_0(\zeta))(z)\|_{\mathcal{B}(\mathcal{H}_t, \mathcal{D})}
\]
\[
\leq C(1 + k^2).
\]
Higher order derivatives, are bounded by the same argument, yielding that \( R_0(\zeta) \) belongs to \( S^m_{\tau}(\mathcal{B}(\mathcal{H}_t, \mathcal{D})) \) uniformly in \( \zeta \). This concludes the induction argument.

From the previous argument it follows moreover that
\[
(\partial_\alpha^\gamma R_j)(\zeta, z) \|_{\mathcal{B}(\mathcal{H}_t, \mathcal{D})} \leq C_{\alpha_j} w(z) \quad \forall \; z \in U_{z_0}, \; \zeta \in \Lambda(z_0) \tag{38}
\]
with \( C_{\alpha_j} \) independent of \( z_0 \in \mathbb{R}^{2d} \). By (38), this implies \( \pi \in M^m_{\tau}(\varepsilon, \mathcal{B}(\mathcal{H}_t, \mathcal{D})) \) and concludes the proof.

**Proof of Proposition 6** From the projector constructed in Lemma 7 one obtains, by resummation, a semiclassical symbol \( \pi \in S^1_{\tau}(\varepsilon, \mathcal{H}_t) \) whose asymptotic expansion is given by \( \sum_{j \geq 0} \varepsilon^j \pi_j \). Then according to Proposition 25 Weyl quantization yields a bounded operator \( \hat{\pi} \in \mathcal{B}(\mathcal{H}_t) \), which is approximately a projector in the sense that
\[
\hat{\pi}^2 = \hat{\pi} + \mathcal{O}_0(\varepsilon^\infty) \quad \text{and} \quad \hat{\pi}^* = \hat{\pi}.
\]

We notice that Proposition 24 implies that \( H \hat{\pi} \in S^m_{\tau}(\varepsilon, \mathcal{B}(\mathcal{H}_t)) \). But \( \tau \)-equivariance implies that the norm is periodic and then \( H \hat{\pi} \pi \) belongs indeed
to \( \mathcal{S}^1(\varepsilon, \mathcal{B}(\mathcal{H}_t)) \). Then \( \tilde{\tau}^* H = (H \tilde{\tau})^* \) belongs to the same class, so that \([H, \pi]^\circ \in \mathcal{S}^1(\varepsilon, \mathcal{B}(\mathcal{H}_t))\). This a priori information on the symbol class, together with Lemma 7.(iii), assures that

\[
[\hat{H}, \hat{\pi}] = \mathcal{O}_0(\varepsilon^\infty)
\]

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

In order to get a true projector, we proceed as in \cite{NeSc}. For \( \varepsilon \) small enough, let

\[
\Pi^\varepsilon := \frac{i}{2\pi} \int_{|\zeta - 1| = \frac{1}{2}} d\zeta (\hat{\pi} - \zeta)^{-1}.
\]

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

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

\[\Box\]

3.2 The intertwining unitaries

After having determined the decoupled subspace associated with an isolated family of Bloch bands, we aim at an effective description of the intraband dynamics, i.e. the dynamics inside this subspace. In order to get a 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 \( \mathcal{K} := L^2(\mathbb{T}^d) \otimes \mathbb{C}\ell \), where \( \ell := \dim P_T(k) \) and \( \mathbb{T}^d \) is \( M^* \) with periodic boundary conditions. Notation will be simpler in the following, if we think of the fibre \( \mathbb{C}\ell \) as a subspace of \( \mathcal{H}_t \). In order to construct such a unitary mapping, we reformulate Assumption (A2).

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

\[
u_0(k, r) \pi_0(k, r) \nu_0^*(k, r) = \pi_r
\]

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

\[
u_0(k + \gamma^*, r) = \nu_0(k, r) \tau(\gamma^*)^{-1},
\]

and \( u_0 \) belongs to \( \mathcal{S}^1(\mathcal{B}(\mathcal{H}_t)) \).

Clearly,

\[
u_0^*(k + \gamma^*, r) = \tau(\gamma^*) \nu_0^*(k, r).
\]

An operator-valued symbol satisfying \( \mathcal{M} \) (resp. \( \mathcal{H} \)) is called left \( \tau \)-covariant (resp. right \( \tau \)-covariant).

The equivalence of (A\(_2\)) and (A\(_2^\prime\)) can be seen as follows. According to Assumption (A\(_2\)), there exists an orthonormal basis \( \{\psi_j(k)\}_{j=1}^\ell \) of \( \text{Ran}P_T(k) \)
which is smooth and τ-equivariant with respect to k. Let πτ := π0(k0, r0) for any fixed point (k0, r0). By the gap condition, dimπτ = dimPτ(k). Then for any orthonormal basis \{χ_j\}_j=1 for Ranπτ, the formula

\[ \tilde{u}_0(k, r) := \sum_{j=1}^{\ell} |χ_j\rangle \langle ψ_j(k - A(r))| \]  

defines a partial isometry which can be extended to a unitary operator \( u_0(k, r) \in \mathcal{U}(\mathcal{H}_1) \). The fact that \( \{ψ_j(k)\}_j=1^{\ell} \) spans Ran\( P_\epsilon(k) \) implies (41), and the τ-equivariance of \( ψ_j(k) \) reflects in (42).

Viceversa, given \( u_0 \) fulfilling Assumption (A2), one can check that the formula

\[ ψ_j(k - A(r)) := u_0^*(k, r)χ_j, \]

with \( \{χ_j\}_j=1^{\ell} \) spanning Ran\( π_\tau \), defines an orthonormal basis for Ran\( P_\epsilon(k) \) which satisfies Assumption (A2).

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 Ran\( \Pi^\epsilon \) to an \( ε \)-independent reference space \( K \subset \mathcal{H}_{ref} \). Since all the twisting of \( \mathcal{H}_\tau \) has been absorbed in the τ-equivariant basis \( \{ψ_j\}_j=1^{\ell} \), or equivalently in \( u_0 \), the space \( \mathcal{H}_{ref} \) can be chosen to be a space of periodic vector-valued functions, i.e.

\[ \mathcal{H}_{ref} := L^2_{\tau=1}(\mathbb{R}^d, \mathcal{H}_\tau) \cong L^2(T^{ds}, \mathcal{H}_\tau). \]

We introduce the orthogonal projector \( \Pi_\tau := \bar{π}_\tau \in \mathcal{B}(\mathcal{H}_{ref}) \) since the effective intraband dynamics can be described in

\[ K := \text{Ran} \Pi_\tau \cong L^2_{\tau=1}(\mathbb{R}^d, \mathbb{C}^\ell) \cong L^2(T^{ds}, \mathbb{C}^\ell) \]

as it will become apparent later on. Recall that \( \ell = \dim P_\epsilon(k) = \dim π_\tau \).

**Proposition 8.** Let \( \{E_n\}_{n \in \mathbb{Z}} \) be an isolated family of bands and let Assumptions (A1) and (A2) be satisfied. Then there exists a unitary operator \( U^\epsilon : \mathcal{H}_\tau \to \mathcal{H}_{ref} \) such that

\[ U^\epsilon \Pi^\epsilon U^\epsilon^* = \Pi_\tau \]

and \( U^\epsilon = \hat{u} + \mathcal{O}(ε^\infty) \), where \( u := \sum_{j \geq 0} ε^j u_j \) belong to \( S^1(ε, \mathcal{B}(\mathcal{H}_\tau)) \), is right τ-covariant at any order and has principal symbol \( u_0 \).

**Proof.** By using the same method as in Lemma 3.3 in [PST1], one constructs first the formal symbol \( \sum_{j \geq 0} ε^j u_j \). Since \( u_0 \) is right τ-covariant, one proves by induction that the same holds true for any \( u_j \). Indeed, by referring to the notation in [PST1], 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 \( b_{n+1} = [π_\tau, B_{n+1}] \). From the defining equation

\[ u^{(n)} \rightleftharpoons u^{(n)*} - 1 = ε^{n+1} A_{n+1} + \mathcal{O}(ε^{n+2}) \]

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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 $\tau$-covariant. Then the defining equation

$$w^{(n)} \not\equiv \pi^\ast w^{(n)} = \pi^\ast = \varepsilon^{n+1} B_{n+1} + O(\varepsilon^{n+2})$$

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

One notices that right $\tau$-covariance is nothing but a special case of $(\tau_1, \tau_2)$-equivariance, for $\tau_2 \equiv 1$ and $\tau_1 = \tau$. Thus it follows from Proposition 29 that the Weyl quantization of $u$ is a bounded operator $\hat{u} \in B(H_{\tau}, H_{\text{ref}})$ such that:

(i) $\hat{u} \hat{u}^\ast = 1_{H_{\text{ref}}} + O_0(\varepsilon^\infty)$ and $\hat{u}^\ast \hat{u} = 1_{H_{\tau}} + O_0(\varepsilon^\infty)$,

(ii) $\hat{u} \Pi^\tau \hat{u}^\ast = \Pi^\tau + O_0(\varepsilon^\infty)$.

Finally we modify $\hat{u}$ as in [PST] by an $O_0(\varepsilon^\infty)$-term in order to get the unitary operator $U^\varepsilon \in U(\tau, H_{\text{ref}})$.

3.3 The effective Hamiltonian

The final step in space-adiabatic perturbation theory is to define and compute the effective Hamiltonian for the intraband dynamics and to compute its lower order terms. This is done, in principle, by projecting the full Hamiltonian $H^\varepsilon_Z$ to the decoupled subspace and afterwards rotating to the reference space.

Proposition 9. Let $\{E_n\}_{n \in \mathbb{Z}}$ be an isolated family of bands and let Assumptions (A1) and (A2) be satisfied. Let $h$ be a resummation in $S^1_{\tau=1}(\varepsilon, B(H))$ of the formal symbol

$$h = u \not\equiv \pi^\ast H \not\equiv \pi^\ast u^\ast \in M^1_{\tau=1}(\varepsilon, B(H))$$

Then $\check{h} \in B(H_{\text{ref}})$, $[\hat{h}, \Pi^\tau] = 0$ and

$$(e^{-iH^\varepsilon_Z t} - U^\varepsilon \ast e^{-i\hat{h} t} U^\varepsilon) \Pi^\tau = O_0(\varepsilon^\infty(1 + |t|)).$$

Remark 10. The definition of the effective Hamiltonian is not entirely unique in the sense that any $H_{\text{eff}}$ satisfying (47) would serve as well as an effective Hamiltonian. However, the asymptotic expansion of $H_{\text{eff}}$ is unique and therefore it is most convenient to define the effective Hamiltonian through (46).

Proof. In the proof we denote $H^\varepsilon_B$ by $\hat{H}$ to emphasize the fact that it is the Weyl quantization of $H \in S^1_{\tau}(\varepsilon, B(D, H))$.

First note that (47) follows from the following facts: according to Lemma 4 and Proposition 24 we have that

$$\pi^\ast H \not\equiv \pi \in M^1_{\tau}(\varepsilon, B(H)) = M^1_{\tau}(\varepsilon, B(H)),$$

where we used that $\tau$ is a unitary representation. With Proposition 8 it follows that $h \in M^1_{\tau=1}(\varepsilon, B(H))$. Therefore $\check{h} \in B(H_{\text{ref}})$ follows from Proposition 25 while $[\hat{h}, \Pi^\tau] = 0$ is satisfied by construction.
It remains to check (47):
\[
(e^{-i\hat{H}t} - U^* e^{-i\hat{H}t} U^*) \Pi^0 = (e^{-i\hat{H}t} - e^{-iU^* \hat{H} U^* t}) \hat{\Pi} + \mathcal{O}_0(\varepsilon^\infty)
\]
\[
= (e^{-i\hat{H}t} - e^{-iU^* \hat{H} U^* t}) \hat{\Pi} + \mathcal{O}_0(\varepsilon^\infty)
\]
\[
= \mathcal{O}(\varepsilon^\infty(1 + |t|)),
\]
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. \(\square\)

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

We compute the principal and the subprincipal symbol of \(\hat{h}\) for the special but most relevant case of an isolated eigenvalue, eventually \(\ell\)-fold degenerate, i.e. \(E_n(k) \equiv E(k)\) for every \(n \in I, |I| = \ell\). Recall that in this special case Assumption \((A_2)\) is equivalent to the existence of an orthonormal system of smooth and \(\tau\)-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 \(\pi_0\) and \(\pi_\tau\) is given by equation (44) where \(\psi_j(k)\) are now Bloch functions, i.e. eigenvectors of \(H_{\text{per}}(k)\) with eigenvalue \(E(k)\).

**Proof of Corollary 4**. In the following \(h\) is identified with \(\pi_\tau h \pi_\tau\) and regarded as a \(\mathcal{B}(\mathcal{C}^\ell)\)-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 (47) follows immediately from the fact that \(h_0 = u_0 H_0 u_0^*\) and that \(\psi_\alpha\) are Bloch functions. As for \(h_1\), we use the general formula of \([\text{PST}_1]\), which reads, transcribed to the present setting, as
\[
h_{1,\alpha\beta}(k, r) = -i \langle \psi_\alpha(\tilde{k}), \{E(\tilde{k}) + \phi(r), \psi_\beta(\tilde{k})\} \rangle - \frac{1}{2} \langle \psi_\alpha(\tilde{k}), \{H_{\text{per}}(\tilde{k}) - E(\tilde{k}), \psi_\beta(\tilde{k})\} \rangle.
\]
(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 (42) while the second term contributes to the \(\alpha\beta\) matrix element with
\[
\frac{1}{2} \sum_{j=1}^{d} \sum_{j=1}^{d} \left( \partial_j A_i - \partial_i A_j \right)(r) \langle \psi_\alpha(\tilde{k}), \partial_i (H_{\text{per}} - E)(\tilde{k}) \partial_j \psi_\beta(\tilde{k}) \rangle_{\hat{H}_t}.
\]
The derivative on \((H_{\text{per}} - E)\) can be moved to the first argument of the inner product by noticing that
\[
0 = \nabla \langle \psi_\alpha, (H_{\text{per}} - E) \phi \rangle = \langle \nabla \psi_\alpha, (H_{\text{per}} - E) \phi \rangle + \langle \psi_\alpha, \nabla (H_{\text{per}} - E) \phi \rangle.
\]
since $\psi_\alpha$ is in the kernel of $(H_{\text{per}} - E)$. Finally the imaginary part of

$$\frac{i}{2} \sum_{j,l=1}^d \left( \partial_j A_l - \partial_l A_j \right)(r) \langle \partial_j \psi_\alpha(\vec{k}), (H_{\text{per}} - E)(\vec{k}) \partial_l \psi_\beta(\vec{k}) \rangle_{\mathcal{H}_t}$$

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

\[\square\]

4 Semiclassical dynamics for Bloch electrons

We have now at our disposal the tools to establish the link between the Schrödinger equation (2) and the corrected semiclassical equations of motion (5). To this end we specialize to the case of a non-degenerate Bloch band $E_n$. The phase space for (5) is $\mathbb{R}^d \times \mathbb{R}^d$, since we use the extended zone scheme, and we denote by $\Phi^t_{\varepsilon}$ the corresponding solution flow. Since the effective Hamiltonian is written in canonical variables, it is necessary to switch in (5) to $(r, k)$ on the “physical” Hilbert space $\mathcal{H}_t$. Let us consider any admissible semiclassical observable $\hat{a}$, and we specialize to the case of a non-degenerate Bloch band $E_n$ be an isolated, non-degenerate Bloch band, see Definition 3 and let the potentials satisfy Assumption (A1). Let $a \in C^\infty_b(\mathbb{R}^{2d})$ be $\Gamma^*$-periodic in the second argument, i.e. $a(r, k + \gamma^*) = a(r, k)$ for all $\gamma^* \in \Gamma^*$, and $\hat{a} = a(\varepsilon x, -i\nabla_x)$ be its Weyl quantization. Then for each finite time-interval $I \subset \mathbb{R}$ there is a constant $C < \infty$ such that for $t \in I$

$$\left\| \Pi^t_{\varepsilon} \left( e^{iH_t/\varepsilon} \hat{a} e^{-iH_t/\varepsilon} - a \circ \Phi^t_{\varepsilon} \right) \right\|_{\mathcal{B}(L^2(\mathbb{R}^d))} \leq \varepsilon^2 C.$$ \hspace{1cm} (49)

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

$$\left| \langle \psi_0, e^{iH_t/\varepsilon} \hat{a} e^{-iH_t/\varepsilon} \psi_0 \rangle - \langle \psi_0, a \circ \Phi^t_{\varepsilon} \psi_0 \rangle \right| \leq \varepsilon^2 C \left\| \psi_0 \right\|^2.$$

Theorem 11 is an Egorov-type theorem, see [Ro]. An unconventional feature is that the first order corrections are treated by considering an $\varepsilon$-dependent Hamiltonian flow instead of having a separate dynamics for the subprincipal symbol of an observable.

By exploiting the relation between Weyl-quantized operators and Wigner transforms, one can easily translate (49) to the language of Wigner functions.
For a detailed discussion on how Theorem 11 relates to alternative approaches to the semiclassical limit in perturbed periodic potentials we refer the reader to [162].

To prove Theorem 11, our strategy is to first establish a corresponding Egorov theorem in the reference space and then to pull back to $L^2(\mathbb{R}^d, dr)$.

**Proposition 12.** Let $E$ be an isolated non-degenerate Bloch band and let $\hat{h}$ be the effective Hamiltonian constructed in Theorem 3, which acts on the reference space $\mathcal{K} = L^2_{r,1}(\mathbb{R}^d)$ of $\Gamma^*$-periodic $L^2_{loc}$-functions. Let $\bar{\Phi}^t : \mathbb{R}^{2d} \rightarrow \mathbb{R}^{2d}$ be the Hamiltonian flow generated by the Hamiltonian function

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

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

$$\left\| e^{i\hat{h}/\varepsilon} \hat{a} e^{-i\hat{h}/\varepsilon} - a \circ \bar{\Phi}^t \right\| \leq C T \varepsilon^2$$

uniformly for any finite interval in time $[-T, T]$.

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

$$e^{i\hat{h}/\varepsilon} \hat{a} e^{-i\hat{h}/\varepsilon} - a \circ \bar{\Phi}^t = \int_0^t \frac{dt'}{dt} \left( e^{i\hat{h}/\varepsilon} (a \circ \bar{\Phi}^{t-t'}) e^{-i\hat{h}/\varepsilon} \right)$$

$$= \int_0^t dt' e^{i\hat{h}/\varepsilon} \left( \frac{i}{\varepsilon} \left[ \hat{h}, (a \circ \bar{\Phi}^{t-t'}) \right] - \left( \frac{d}{dt'} (a \circ \bar{\Phi}^{t-t'}) \right)^\wedge \right) e^{-i\hat{h}/\varepsilon},$$

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

$$\frac{d}{dt'} (a \circ \bar{\Phi}^{t-t'}) = \{ h_{cl}, a \circ \bar{\Phi}^{t-t'} \}$$

and, computing the expansion of the Moyal product,

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

In order to obtain the Egorov theorem for the physical observables, we need to undo the transform to the reference space and the Zak transform. We start with the simpler observation on how the Zak transform maps semiclassical observables.
Proposition 13. Let $a \in S^1(\varepsilon, \mathbb{C})$ be $\Gamma^*$-periodic, i.e. $a(r, k + \gamma^*) = a(r, k)$ for all $\gamma^* \in \Gamma^*$. Let $b(k, r) = a(r, k)$ then $b \in S^1\gamma(\varepsilon, \mathbb{C})$ and

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

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

Remark 14. An analogous statement cannot be true for general operator-valued $\tau$-equivariant symbols. For example, the symbol $b(k, r) := H_{\text{per}}(k - A(r))$ is $\tau$-equivariant and in particular a semiclassical observable. However, the corresponding operator in the original representation is

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

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

Proof. We give the proof for $a(\cdot, k) \in \mathcal{S}(\mathbb{R}^d)$. The general result follows from standard density arguments, see [DiS]). For $\psi \in \mathcal{S}(\mathbb{R}^d)$ we have according to (11) the explicit formula

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

(51)

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

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

(52)

The assumptions on $a$ and $\psi$ 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 Zak transform of (52) using (11).

$$(U^{-1}\widehat{b} \varphi)(x) =$$

(53)

$$= \sum_{\gamma \in \Gamma} \int_{B} dk \int_{\mathbb{R}^d} d\eta(\mathcal{F}b)(\gamma, \eta) \ e^{ik \cdot x} e^{-i(\eta \cdot \gamma)/2} e^{i\varepsilon \gamma \cdot k} \varphi(k - \varepsilon \eta, [x])$$

$$= \sum_{\gamma \in \Gamma} \int_{B} d\eta(\mathcal{F}b)(\gamma, \eta) e^{i(\gamma \cdot x)/2} e^{i\varepsilon \gamma \cdot x} \int_{M^*} dk e^{i(k - \varepsilon \eta) \cdot (x + \gamma)} \varphi(k - \varepsilon \eta, [x]).$$

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

$$\int_{M^*} dk e^{i(k - \varepsilon \eta) \cdot (x + \gamma)} \varphi(k - \varepsilon \eta, [x]) = \int_{M^*} dk e^{ik \cdot (x + \gamma)} \varphi(k, [x + \gamma]) = \psi(x + \gamma).$$

Inserting this expression in the last line of (53) and comparing with (51) concludes the proof. \[\square\]
Before we arrive at the proof of Theorem 11, one has to study how the unitary map constructed in Section 3.2 maps observables in the Zak representation to observables in the reference representation.

**Proposition 15.** Let \( \tilde{b} = b_0(k, \varepsilon i \nabla_k) + \varepsilon b_1(k, \varepsilon i \nabla_k) \) with symbol \( b \in S^1(\varepsilon, \mathbb{C}) \) which is \( \Gamma^* \)-periodic in the first argument. Let \( U^\varepsilon : \Pi^\varepsilon \mathcal{H}_\tau \to \mathcal{K} \) be the unitary map constructed in Section 3.2. Then

\[
U^\varepsilon \Pi^\varepsilon \tilde{b} \Pi^\varepsilon U^{\varepsilon*} = \tilde{c} + \mathcal{O}(\varepsilon^2),
\]

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

\[
T : \mathbb{R}^{2d} \to \mathbb{R}^{2d}, \quad (k, r) \mapsto \left( k + \varepsilon A_m(k - A(r)) \nabla A_m(r), \, r + \varepsilon A(k - A(r)) \right).
\]

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

**Proof.** In order to compute \( c = u \varepsilon \pi \tilde{b} \pi u^* \), observe that, since \( b \) is scalar-valued, the principal symbol remains unchanged, i.e. \( c_0 = u_0 \tau_0 b_0 \tau_0 u_0^* = b_0 \). For the subprincipal symbol we use the general transformation formula obtained for the Hamiltonian, which applies to all operators whose principal symbol commutes with \( \pi_0 \). In this case the eigenvalue \( E \) in (18) must be replaced by the corresponding principal symbol and a term for the subprincipal symbol \( b_1 \) must be added. Hence we find that

\[
c_1(k, r) = -i \langle \psi(k - A(r)), \{ b_0(k, r), \psi(k - A(r)) \} \rangle \\
+ \langle \psi(k - A(r)), b_1(k, r) \psi(k - A(r)) \rangle \\
= \partial_{k_n} b_0(k, r) i \langle \psi(k - A(r)), \partial_{r_n} \psi(k - A(r)) \rangle \partial_{r_n} A_m(r) \\
+ \partial_{r_n} b_0(k, r) i \langle \psi(k - A(r)), \partial_{k_n} \psi(k - A(r)) \rangle + b_1(k, r) \\
= \partial_{k_n} b_0(k, r) A_m(k - A(r)) \partial_{r_n} A_m(r) \\
+ \partial_{r_n} b_0(k, r) A_m(k - A(r)) + b_1(k, r),
\]

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

We have now all the ingredients needed for the

**Proof of Theorem 11.** Let \( a \in C^\infty(\mathbb{R}^{2d}) \) be \( \Gamma^* \)-periodic in the second argument, then according to Proposition 15, we have

\[
\Pi_n^\varepsilon e^{i H^{\varepsilon t} / \varepsilon} \tilde{a} e^{-i H^{\varepsilon t} / \varepsilon} = \mathcal{U}^* \Pi^\varepsilon e^{i H_2^{\varepsilon t} / \varepsilon} \tilde{b} e^{-i H_2^{\varepsilon t} / \varepsilon} \Pi^\varepsilon \mathcal{U}
\]

with \( b(k, r) = a(r, k) \). With Theorem 9 and Proposition 15, we find that

\[
\Pi^\varepsilon e^{i H_2^{\varepsilon t} / \varepsilon} \tilde{b} e^{-i H_2^{\varepsilon t} / \varepsilon} \Pi^\varepsilon = U^\varepsilon a \tilde{c} e^{-i \tilde{c} \mathcal{U} t / \varepsilon} U^\varepsilon + \mathcal{O}(\varepsilon^2),
\]

where \( c(\varepsilon, k, r) = (b \circ T)(k, r) \). Now we can apply Proposition 12 to conclude that

\[
e^{-i \tilde{c} \mathcal{U} t / \varepsilon} \tilde{c} e^{-i \tilde{c} \mathcal{U} t / \varepsilon} = (c \circ \Phi^t) + \mathcal{O}(\varepsilon^2).
\]
Since, for $\varepsilon$ sufficiently small, $T$ is a diffeomorphism, one can write
\[ c \circ \tilde{\Phi}^t = c \circ T^{-1} \circ T \circ \tilde{\Phi}^t \circ T^{-1} \circ T =: c \circ T^{-1} \circ \Phi^t \circ T = b \circ \Phi^t \circ T, \]
where the flow $\Phi^t$ in the new coordinates will be computed explicitly below. Inserting the results into (55), one obtains
\[ \Pi^\varepsilon e^{iH^t/\varepsilon} \tilde{b} e^{-iH^t/\varepsilon} \Pi^\varepsilon = U^\varepsilon \ast (b \circ \Phi^t \circ T) U^\varepsilon + O(\varepsilon^2) \]
\[ = \Pi^\varepsilon (b \circ T) \Pi^\varepsilon + O(\varepsilon^2), \]
where we used Proposition 15 for the second equality. Inserting into (54) we finally find that
\[ \Pi^\varepsilon e^{iH^t/\varepsilon} \tilde{a} e^{-iH^t/\varepsilon} \Pi^\varepsilon = \Pi^\varepsilon (a \circ \Phi^t) \Pi^\varepsilon + O(\varepsilon^2), \quad (56) \]
where we did not make the exchange of the order of the arguments in $a$ explicit.

Since the flow is determined only in approximation and only through its vector field, we make use of the following lemma.

**Lemma 16.** Let $\Phi_i : \mathbb{R}^{2d} \times \mathbb{R} \to \mathbb{R}^{2d}$ be the flow associated with the vector field $v_i \in C^\infty_b(\mathbb{R}^{2d}, \mathbb{R}^{2d}), i = 1, 2$.

(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
\[ \sup_{t \in I, x \in \mathbb{R}^{2d}} |\partial^\alpha (\Phi^t_1 - \Phi^t_2)(x)| \leq C_{I, \alpha} \varepsilon^2. \quad (57) \]

(ii) Let $a \in S^1(\varepsilon, \mathbb{C})$. If (57) holds for the flows $\Phi_1, \Phi_2$, then there is a constant $C < \infty$, such that for all $t \in I$
\[ \|a \circ \Phi^t_1 - a \circ \Phi^t_2\|_{B(L^2(\mathbb{R}^d)))} \leq C \varepsilon^2. \]

**Proof.** Assertion (i) is 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 $O(\varepsilon^2)$ according to (57).

According to assertion (ii) of the lemma it suffices to show that
\[ \Phi^t_1(r, k) = \left( \Phi^t_{e^r}(r, k - A(r)), \Phi^t_{e^r}(r, k - A(r)) + A(r) \right) + O(\varepsilon^2) \]
in the above sense, where $\Phi^t_1$ is the flow of (55). 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 $\Phi_t^t$ up to an error of order $O(\varepsilon^2)$. We start with the vector field of $\Phi_t^t$. The effective Hamiltonian on the reference space including first order terms reads

$$h(r, k) = E(k - A(r)) + \phi(r)$$

(58)

$$- \varepsilon \left( F_{\text{Lor}}(r, \nabla E(k - A(r))) \cdot A(k - A(r)) + B(r) \cdot M(k - A(r)) \right),$$

with the Lorentz force

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

Componentwise, the canonical equations of motion are

$$\dot{r}_j = \partial_{k_j} h(r, k) = \partial_{k_j} E(k - A(r))$$

$$- \varepsilon \partial_{k_j} \left( F_{\text{Lor}}(r, k - A(r)) \cdot A(k - A(r)) + B(r) \cdot M(k - A(r)) \right),$$

$$\dot{k}_j = -\partial_{r_j} h(r, k) = -\partial_{r_j} \phi(r) + \partial_t E(k - A(r)) \partial_{j} A_t(r)$$

$$- \varepsilon \partial_{k_j} \left( A(k - A(r)) \cdot F_{\text{Lor}}(r, k - A(r)) + B(r) \cdot M(k - A(r)) \right) \partial_{j} A_t(r)$$

$$- \varepsilon A_t(k - A(r)) \left( \partial_{j} \partial_{r} \phi(r) - (\nabla E(k - A(r)) \times \partial_{j} B(r)) \right)$$

$$+ \varepsilon \partial_{j} B(r) \cdot M(k - A(r)),$$

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

$$\dot{r}_j = \partial_{j} E(\tilde{k}) - \varepsilon \partial_{k_j} \left( F_{\text{Lor}}(\tilde{r}, \tilde{k}) \cdot A(\tilde{k}) + B(r) \cdot M(\tilde{k}) \right)$$

and

$$\dot{k}_j = \dot{\tilde{k}}_j - \partial_{t} A_{j}(r) \dot{\tilde{r}}_t$$

$$= -\partial_{j} \phi(r) + \partial_t E(\tilde{k}) \partial_{j} A_t(r)$$

$$- \varepsilon \partial_{k_j} \left( A(\tilde{k}) \cdot F_{\text{Lor}}(r, \tilde{k}) + M(\tilde{k}) \cdot B(r) \right) \partial_{j} A_t(r)$$

$$+ \varepsilon A_t(\tilde{k}) \partial_{j} F_{\text{Lor}}(r, \tilde{k}) + \varepsilon \partial_{j} B(r) \cdot M(\tilde{k})$$

$$= -\partial_{j} \phi(r) + \dot{\tilde{r}}_t \left( \partial_{j} A_t(r) - \partial_t A_j(r) \right)$$

$$+ \varepsilon A_t(\tilde{k}) \partial_{j} F_{\text{Lor}}(r, \tilde{k}) + \varepsilon \partial_{j} B(r) \cdot M(\tilde{k}),$$

which, in more compact form, read

$$\dot{r} = \nabla E(\tilde{k}) - \varepsilon \nabla_{\tilde{k}} \left( A(\tilde{k}) \cdot F_{\text{Lor}}(r, \tilde{k}) + B(r) \cdot M(\tilde{k}) \right),$$

(59)

$$\dot{\tilde{k}} = -\nabla \phi(r) + \dot{\tilde{r}} \times B(r) + \varepsilon \nabla_{\tilde{r}} \left( A(\tilde{k}) \cdot F_{\text{Lor}}(r, \tilde{k}) + B(r) \cdot M(\tilde{k}) \right).$$
As the next step we perform the change of coordinates induced by $T$, 

$$q = r + \varepsilon A(k), \quad p = \tilde{k} - A(r) + \varepsilon \nabla_r \left( A(k) \cdot A(r) \right),$$  

and then switch to the kinetic momentum

$$v = \frac{p - A(q)}{k + \varepsilon A_l(k) \nabla A_l(r) - \varepsilon A_i(k) \partial_i A(r) + O(\varepsilon^2)}$$

where we used Taylor expansion. The inverse transformations are

$$r = q - \varepsilon A(v) + O(\varepsilon^2),$$

$$\tilde{k} = v - \varepsilon A(v) \times B(q) + O(\varepsilon^2).$$

Recall that we want to show that $(q,v)$ satisfy the semiclassical equations of motion (5), where $q$ is identified with $r$ and $v$ with $\kappa$. The new notation is introduced here, only to make a clear distinction between the canonical variables $(r,k)$ in the reference representation and the canonical variables $(q,p)$ in the original representation.

We now substitute (60) and (61). In the following computations we use several times Taylor expansion to first order and drop terms of order $\varepsilon^2$. In particular in the terms of order $\varepsilon$ one can replace $r$ by $q$ and $\tilde{k}$ by $v$. We find

$$\dot{q}_j = \dot{r}_j + \dot{\varepsilon} \dot{A}_j(v)$$

$$= \partial_j E(v) - \varepsilon \left( A(v) \times B(q) \right)_l \partial_l \partial_j E(v)$$

$$- \varepsilon \partial_j \left( \left( - \nabla \phi(q) + \nabla E(v) \times B(q) \right)_l A_l(v) + B(q) \cdot M(v) \right)$$

$$+ \varepsilon \partial_l A_j(v)$$

$$= \partial_j E(v) - \varepsilon \dot{v}_l \left( \partial_j A_l - \partial_l A_j \right) - \varepsilon B(q) \cdot \partial_j M(v)$$

$$= \partial_j E(v) - \varepsilon v \cdot \Omega(v) \right)_j - \varepsilon B(q) \cdot \partial_j M(v),$$

where it is used that $\dot{v} = F_{\text{Lett}} + O(\varepsilon)$. Thus we obtained the first equation of (5). For the second equation we find

$$\dot{v}_j = \dot{k}_j + \varepsilon \frac{d}{dt} \left( A(v) \times B(q) \right)$$

$$= - \partial_j \phi(q) + \varepsilon A_l(v) \partial_l \partial_j \phi(q)$$

$$+ \left( \dot{q} \times B(q) \right)_j - \varepsilon \left( A(v) \times B(q) \right)_j - \varepsilon \left( \dot{q} \times (A_i(v) \partial_i B(q)) \right)_j$$

$$+ \varepsilon A(u) \partial q \cdot F_{\text{Lett}}(q,v) + \varepsilon \partial_j B(q) \cdot M(v)$$

$$+ \varepsilon \left( A(v) \times B(q) \right)_j + \varepsilon \left( A(v) \times (\dot{q} \partial_i B(q)) \right)_j$$

$$= - \partial_j \phi(q) + \left( \dot{q} \times B(q) \right)_j + \varepsilon \partial_j B(q) \cdot M(v),$$
where the term
\[
\varepsilon \mathcal{A}(v) \left( \partial_q F_{\text{Lor}}(q,v) + \partial_l \partial_j \phi(q) \right) = \varepsilon \mathcal{A}(v) \left( \dot{q} \times \partial_j B(q) \right) + \mathcal{O}(\varepsilon^2)
\]
cancels the remaining two terms. Changing back notation from \((q,v)\) to \((r,\kappa)\), this concludes the proof of Theorem 11. 

\[\square\]

## A Operator-valued Weyl calculus for \(\tau\)-equivariant symbols

The pseudodifferential calculus for scalar-valued symbols defined on the phase space \(T^*\mathbb{R}^d = \mathbb{R}^{2d}\) can be translated to the phase space \(T^*T^d = T^d \times \mathbb{R}^d\), a flat torus, by restricting to periodic functions and symbols. This approach is used by Gérard and Nier [GeNi] in the context of scattering theory in periodic media.

In this appendix we present a similar approach to Weyl quantization of operator-valued symbols which are not exactly periodic, but \(\tau\)-equivariant with respect to some nontrivial representation \(\tau\) of the group of lattice translations. We obtain a pseudodifferential and semiclassical calculus which can be applied to \(\tau\)-equivariant symbols like the Schrödinger Hamiltonian with periodic potential in the Zak 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 \(\tau\)-equivariant in the configurational variable.

Let \(\Gamma \subset \mathbb{R}^d\) be a regular lattice generated through the basis \(\{\gamma_1, \ldots, \gamma_d\}\), \(\gamma_j \in \mathbb{R}^d\), i.e.
\[\Gamma = \left\{ x \in \mathbb{R}^d : x = \sum_{j=1}^{d} \alpha_j \gamma_j \text{ for some } \alpha \in \mathbb{Z}^d \right\}.\]

Clearly the translations on \(\mathbb{R}^d\) by elements of \(\Gamma\) form an abelian group isomorphic to \(\mathbb{Z}^d\). The centered fundamental cell of \(\Gamma\) is denoted as
\[M = \left\{ x \in \mathbb{R}^d : x = \sum_{j=1}^{d} \alpha_j \gamma_j \text{ for } \alpha_j \in [-\frac{1}{2}, \frac{1}{2}] \right\}.
\]

Let \(\mathcal{H}\) be a separable Hilbert space and let \(\tau\) be a representation of \(\Gamma\) in \(B^*(\mathcal{H})\), the group of invertible elements of \(B(\mathcal{H})\) , i.e. a group homomorphism
\[\tau : \Gamma \to B^*(\mathcal{H}), \quad \gamma \mapsto \tau(\gamma).
\]
If more than one Hilbert space appears, then \(\tau\) 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 \(\Gamma\) corresponds to the dual lattice \(\Gamma^\ast\) in momentum space \(\mathbb{R}^d\).

Let \(L_\gamma\) 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 17. A tempered distribution \( T \in \mathcal{S}'(\mathbb{R}^d, \mathcal{H}) \) is said to be \( \tau \)-equivariant if
\[
L_{\gamma}T = \tau(\gamma)T \quad \text{for all } \gamma \in \Gamma,
\]
where \( \tau(\gamma)T(\varphi) = T(\tau(\gamma)^{-1}\varphi) \) for \( \varphi \in \mathcal{S}(\mathbb{R}^d, \mathcal{H}) \). The subspace of \( \tau \)-equivariant distributions is denoted as \( \mathcal{S}'_{\tau} \). Analogously we define
\[
\mathcal{H}_{\tau} = \left\{ \psi \in L^2_{\text{loc}}(\mathbb{R}^d, \mathcal{H}) : \psi(x - \gamma) = \tau(\gamma)\psi(x) \quad \text{for all } \gamma \in \Gamma \right\},
\]
which, equipped with the inner product
\[
\langle \varphi, \psi \rangle_{\mathcal{H}_{\tau}} = \int_M \langle \varphi(x), \psi(x) \rangle_{\mathcal{H}}
\]
is a Hilbert space. Clearly
\[
C^\infty_{\tau} = \left\{ \psi \in C^\infty(\mathbb{R}^d, \mathcal{H}) : \psi(x - \gamma) = \tau(\gamma)\psi(x) \quad \text{for all } \gamma \in \Gamma \right\},
\]
is a dense subspace of \( \mathcal{H}_{\tau} \). \( \diamond \)

Notice that if \( \tau \) 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 \( \tau \)-equivariant functions, we define \( \tau \)-equivariant symbols. To this end we first recall the definition of the standard symbol classes.

Definition 18. 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 \( x, y \in \mathbb{R}^{2d} \). \( \diamond \)

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

Definition 19. A function \( A \in C^\infty(\mathbb{R}^{2d}, B(\mathcal{H}_1, \mathcal{H}_2)) \) 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
\[
\left\| (\partial_q^\alpha \partial_p^\beta A)(q, p) \right\|_{B(\mathcal{H}_1, \mathcal{H}_2)} \leq C_{\alpha, \beta} w(q, p) \tag{62}
\]
for every \( q, p \in \mathbb{R}^d \). \( \diamond \)

Definition 20. 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
\[
A \asymp \sum_{j=0}^{\infty} \varepsilon^j A_j \quad \text{in } S^w(\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)).
\]
distributional integral kernel usual Weyl quantization

\[ A_{\tau} \]

Definition 21. A symbol \( A_\tau \in S^w(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)) \) is \( \tau \)-equivariant (more precisely \((\tau_1, \tau_2)\)-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 \( \tau \)-equivariant symbols is denoted as \( S^w_\tau(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)) \).

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

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

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

Notice that integral kernel associated to a \( \tau \)-equivariant symbol \( A \) is \( \tau \)-equivariant in the following sense:

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

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

Proposition 22. Let \( A \in S^w_\tau(\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)) \), then

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

Proof. Since \( \tilde{A} \) maps \( S'(\mathbb{R}^d, \mathcal{H}_1) \) continuously into \( S'(\mathbb{R}^d, \mathcal{H}_2) \), we only need to show that \( (L_\gamma \tilde{A} T)(\varphi) = \tau_2(\gamma) \tilde{A} T(\varphi) \) for all \( T \in S'_{\tau_1}(\mathbb{R}^d, \mathcal{H}_1) \) 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 \( [\tilde{A}, L_\gamma T] = L_\gamma (\tau_1(\gamma)^{-1})^* \tilde{A} T \tau_2(\gamma)^* \). Indeed, let \( \psi \in \mathcal{S}(\mathbb{R}^d, \mathcal{H}_2) \) be
Hence, using the fact that \( \tau \) is a representation and that \( L_\gamma T = \tau_1(\gamma)T \),

\[
(L_\gamma \tilde{A} T)(\varphi) = T(\tilde{A}^* L_{-\gamma} \varphi) = T(L_{-\gamma} \tau_1(\gamma)^* \tilde{A}^* (\tau_2(\gamma)^{-1})^* \varphi) = (\tau_2(\gamma) \tilde{A} \tau_1(\gamma)^{-1} L_\gamma T)(\varphi) = (\tau_2(\gamma) \tilde{A} T)(\varphi).
\]

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. [DIS].

**Proposition 23.** 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 \( \tilde{A}B = \tilde{C} \), with \( C \in S^{w_1+w_2}(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_3)) \) given through

\[
C(\varepsilon, q, p) = \exp \left( \frac{i \varepsilon}{2} (\nabla_p \cdot \nabla_\xi - \nabla_\xi \cdot \nabla_q) \right) A(\varepsilon, q, p)B(\varepsilon, x, \xi)|_{x=q, \xi=p} =: A\tilde{\times}B.
\]

(66)

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

\[
\tilde{\times} : M^{w_1}(\varepsilon, \mathcal{B}(\mathcal{H}_2, \mathcal{H}_3)) \times M^{w_2}(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)) \to M^{w_1+w_2}(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_3)).
\]

The \( \tau \)-equivariance of symbols is preserved under the pointwise product, the Weyl product and the Moyal product.

**Proposition 24.** Let \( A_\varepsilon \in S^{w_1}(\varepsilon, \mathcal{B}(\mathcal{H}_2, \mathcal{H}_3)) \) and \( B_\varepsilon \in S^{w_2}(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)) \), then \( A_\varepsilon B_\varepsilon \in S^{w_1+w_2}(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_3)) \) and \( A_\varepsilon \tilde{\times} B_\varepsilon \in S^{w_1+w_2}(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_3)) \).

**Proof.** One has

\[
A_\varepsilon(q - \gamma, p)B_\varepsilon(q - \gamma, p) = \tau_3(\gamma)A_\varepsilon(q, p)\tau_2(\gamma)^{-1}\tau_2(\gamma)B_\varepsilon(q, p)\tau_1(\gamma)^{-1} = \tau_3(\gamma)A_\varepsilon(q, p)B_\varepsilon(q, p)\tau_1(\gamma)^{-1},
\]

which shows \( A_\varepsilon B_\varepsilon \in S^{w_1+w_2}(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_3)) \) and inserted into (66) yields immediately also \( A_\varepsilon \tilde{\times} B_\varepsilon \in S^{w_1+w_2}(\varepsilon, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_3)) \).

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 25. Let \( A \in S^1_1(\mathcal{B}(\mathcal{H})) \) and \( \tau_1, \tau_2 \) unitary representations of \( \Gamma \) in \( \mathcal{B}(\mathcal{H}) \), then \( \hat{A} \in \mathcal{B}(\mathcal{H}_{\tau_1}, \mathcal{H}_{\tau_2}) \) and for \( A_\varepsilon \in S^1_1(\varepsilon, \mathcal{B}(\mathcal{H})) \) we have that
\[
\sup_{\varepsilon \in [0, \varepsilon_0]} \| \hat{A}_\varepsilon \|_{\mathcal{B}(\mathcal{H}_{\tau_1}, \mathcal{H}_{\tau_2})} < \infty.
\]

Proof. Fix \( n > d/2 \) and let \( w(x) = \langle x \rangle^{-n} \). We consider the weighted \( L^2 \)-space
\[
L^2_w = \left\{ \psi \in L^2_{\text{loc}}(\mathbb{R}^d, \mathcal{H}) : \int_{\mathbb{R}^d} dx w(x)^2 \| \psi(x) \|^2 < \infty \right\}.
\]

Let \( j = 1, 2 \), then \( \mathcal{H}_{\tau_j} \subset L^2_w \) and for any \( \psi \in \mathcal{H}_{\tau_j} \) one has the norm equivalence
\[
C_1 \| \psi \|_{\mathcal{H}_{\tau_j}} \leq \| \psi \|_{L^2_w} \leq C_2 \| \psi \|_{\mathcal{H}_{\tau_j}} \quad (67)
\]
for appropriate constants \( 0 < C_1, C_2 < \infty \). The first inequality in (67) is obvious and the second one follows by exploiting \( \tau_j \)-equivariance of \( \psi \) and unitarity of \( \tau_j \):
\[
\| \psi \|_{L^2_w}^2 = \sum_{\gamma \in \Gamma} \int_{M + \gamma} dx w(x)^2 \| \tau_j(\gamma)^{-1} \psi(x) \|_{\mathcal{H}}^2 = \sum_{\gamma \in \Gamma} \int_{M + \gamma} dx w(x)^2 \| \psi(x) \|_{\mathcal{H}}^2 \leq \sum_{\gamma \in \Gamma} \sup_{x \in M + \gamma} \{ w(x)^2 \} \int_M dx \| \psi(x) \|_{\mathcal{H}}^2 \leq C_2 \| \psi \|_{\mathcal{H}_{\tau_j}}.
\]

According to (67) it suffices to show that \( \hat{A} \in \mathcal{B}(L^2_w) \) and to estimate the norm of \( \hat{A} \) in this space.

Let \( \psi \in C^\infty_{\text{loc}}(\mathbb{R}^d, \mathcal{H}) \), then by the general theory \( \hat{A} \psi \) is smooth as well (see [150], Corollary 2.62) and thus, according to Proposition [120], \( \hat{A} \psi \in C^\infty_{\text{loc}}(\mathbb{R}^d, \mathcal{H}) \). Hence we can use (67) and find
\[
\| \hat{A} \psi \|_{L^2_w} = \| w^{1/2} \hat{A} \psi \|_{L^2_w} \leq \| w^{1/2} \hat{A} w^{-1} \|_{\mathcal{B}(L^2_w)} \| \psi \|_{L^2_w} = \| w^{1/2} \hat{A} w^{-1} \|_{\mathcal{B}(L^2_w)} \| \psi \|_{L^2_w}.
\]

However, by Proposition [120] we have that \( w^{1/2} \hat{A} w^{-1} \in S^1(\varepsilon, \mathcal{B}(\mathcal{H})) \). Thus from the usual Calderon-Vaillancourt theorem it follows that
\[
\| w^{1/2} \hat{A} w^{-1} \|_{\mathcal{B}(L^2)} \leq C_d \| w^{1/2} A_\varepsilon w^{-1} \|_{C^{2d+1}_{\text{b}}(\mathbb{R}^d)}.
\]

This shows that for \( A \in S^1_1(\mathcal{B}(\mathcal{H})) \) we have \( \hat{A} \in \mathcal{B}(\mathcal{H}_{\tau_1}, \mathcal{H}_{\tau_2}) \). With \( w^{1/2} A_\varepsilon w^{-1} \in S^1(\varepsilon, \mathcal{B}(\mathcal{H})) \) for \( A_\varepsilon \in S^1_1(\varepsilon, \mathcal{B}(\mathcal{H})) \), we conclude that
\[
\sup_{\varepsilon \in [0, \varepsilon_0]} \| \hat{A}_\varepsilon \|_{\mathcal{B}(\mathcal{H}_{\tau_1}, \mathcal{H}_{\tau_2})} < \infty
\]
by the same argument. \( \Box \)

Remark 26. It is clear from the proof that the previous result still holds true under the weaker assumption that \( \tau_1 \) and \( \tau_2 \) are uniformly bounded, i.e. that
\[
\sup_{\gamma \in \Gamma} \| \tau_j(\gamma) \|_{\mathcal{B}(\mathcal{H})} \leq C_j, \quad j = 1, 2.
\]
Finally we would also like to show that for \( A \in S^1_1(B(H)) \) the adjoint of \( \hat{A} \) as an operator in \( B(H_\tau) \), denoted by \( \hat{A}^\dagger \), is given through the quantization of the pointwise adjoint, i.e. through \( \hat{A}^* \). Here it is crucial that \( \tau \) is a unitary representation.

**Proposition 27.** Let \( S^1_1(B(H)) \) with a unitary representation \( \tau \) (with \( \tau_1 = \tau_2 = \tau \)) and let \( \hat{A}^\dagger \) be the adjoint of \( \hat{A} \in B(H_\tau) \), then \( \hat{A}^\dagger = \hat{A}^* \).

**Proof.** Let \( \psi \in H_\tau \) and \( \varphi \in C^\infty_0(\mathbb{R}^d, H) \) such that 
\[
\tilde{\varphi} := \mathbb{1}_M \varphi \in C^\infty_0(\mathbb{R}^d, H),
\]
where \( \mathbb{1}_M \) denotes the characteristic function of the set \( M \). Such \( \varphi \) are dense in \( H_\tau \) and the corresponding \( \tilde{\varphi} \) can be used as a test function:

\[
\langle \varphi, \hat{A}\psi \rangle_{H_\tau} = \int_M dx \langle \varphi(x), (\hat{A}\psi)(x) \rangle_{H_\tau} = \int_{\mathbb{R}^d} dx \langle \tilde{\varphi}(x), (\hat{A}\psi)(x) \rangle_{H_\tau}
\]

\[
= \int_{\mathbb{R}^d} dx \langle (\hat{A}^*\tilde{\varphi})(x), \psi(x) \rangle_{H_\tau}
\]

\[
= \int_{\mathbb{R}^d} dx \langle \int_{\mathbb{R}^d} dy K_A^*(x,y)\tilde{\varphi}(y), \psi(x) \rangle_{H_\tau}
\]

\[
= \int_{\mathbb{R}^d} dx \int_{\mathbb{R}^d} dy K_A^*(x,y)\tilde{\varphi}(y), \psi(x) \rangle_{H_\tau}
\]

\[
= \int_{\mathbb{R}^d} dx \sum_{\gamma \in \Gamma} \langle \int_{M} dy K_A^*(x + \gamma, y)\tilde{\varphi}(y), \psi(x + \gamma) \rangle_{H_\tau}
\]

\[
= \int_{\mathbb{R}^d} dx \sum_{\gamma \in \Gamma} \langle \int_{M} dy \tau^{-1}(\gamma)K_A^*(x, y - \gamma)\tilde{\varphi}(y), \tau\psi(x) \rangle_{H_\tau}
\]

\[
= \int_{\mathbb{R}^d} dx \sum_{\gamma \in \Gamma} \langle \int_{M} dy K_A^*(x, y - \gamma)\tilde{\varphi}(y), \psi(x) \rangle_{H_\tau}
\]

\[
= \int_{\mathbb{R}^d} dx \langle (\hat{A}^*\varphi)(x), \psi(x) \rangle_{H_\tau} = \langle \hat{A}^*\varphi, \psi \rangle_{H_\tau}.
\]

In particular, we used the \( \tau \)-equivariance of the kernel (65) and of the functions in \( H_\tau \) and the unitarity of \( \tau \). By density we have \( \hat{A}^* = \hat{A}^\dagger \).

**B Hamiltonian formulation for the refined semiclassical model**

The dynamical equations (5), which define the \( \varepsilon \)-corrected semiclassical model, can be written as

\[
\dot{r} = \nabla_\kappa H_{sc}(r, \kappa) - \varepsilon \dot{\kappa} \times \Omega_{\kappa}(\kappa),
\]

\[
\dot{\kappa} = -\nabla_\tau H_{sc}(r, \kappa) + \dot{r} \times B(r)
\]
with
\[ H_{sc}(r, \kappa) := E_n(\kappa) + \phi(r) - \varepsilon M_n(\kappa) \cdot B(r). \]

Recall that we are using the notation introduced in Remark and that \( B \) and \( \Omega_n \) are the 2-forms corresponding to the magnetic field and to the curvature of the Berry connection, i.e. in components
\[ B(r)_{ij} = (\partial_i A_j - \partial_j A_i)(r) \]
for \( i, j \in \{1, \ldots, d\} \), and
\[ \Omega_n(\kappa)_{ij} = (\partial_i \mathcal{A}_j - \partial_j \mathcal{A}_i)(\kappa). \]

We fix the system of coordinates \( z = (r, \kappa) \) in \( \mathbb{R}^{2d} \). The standard symplectic form \( \Theta_0 = \Theta_0(z)_{lm} \, dz_m \wedge dz_l \), where \( l, m \in \{1, \ldots, 2d\} \), has coefficients given by the constant matrix
\[ \Theta_0(z) = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}, \]
where \( I \) is the identity matrix in \( \text{Mat}(d, \mathbb{R}) \). The symplectic form, which turns \( \Theta_{B, \varepsilon} \) into Hamilton’s equation of motion for \( H_{sc} \), is given by the 2-form \( \Theta_{B, \varepsilon} = \Theta_{B, \varepsilon}(z)_{lm} \, dz_m \wedge dz_l \) with coefficients
\[ \Theta_{B, \varepsilon}(r, \kappa) = \begin{pmatrix} B(r) & -I \\ I & \varepsilon \Omega_n(\kappa) \end{pmatrix}. \]

For \( \varepsilon = 0 \) the 2-form \( \Theta_{B, \varepsilon} \) coincides with the magnetic symplectic form \( \Theta_B \) usually employed to describe in a gauge-invariant way the motion of a particle in a magnetic field ([MaRa], Section 6.6). For \( \varepsilon \) small enough, the matrix \( \Theta_{B, \varepsilon} \) defines a symplectic form, i.e. a closed non-degenerate 2-form. Indeed, since \( \det \Theta_B = 1 \) it follows that, for \( \varepsilon \) small enough, \( \Theta_{B, \varepsilon} \) is not degenerate. In particular it is sufficient to choose
\[ \varepsilon < \sup_{r, \kappa \in \mathbb{R}^d} \left( \| B(r) \Omega_n(\kappa) \| + \| \Omega_n(\kappa) \| \right). \]

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

With these definitions the corresponding Hamiltonian equations are
\[ \Theta_{B, \varepsilon}(z) \frac{\dot{z}}{} = dH_{sc}(z), \]
or equivalently
\[ \begin{pmatrix} B(r) & -I \\ I & \varepsilon \Omega_n(\kappa) \end{pmatrix} \begin{pmatrix} \dot{r} \\ \dot{\kappa} \end{pmatrix} = \begin{pmatrix} \nabla_r H(r, \kappa) \\ \nabla_\kappa H(r, \kappa) \end{pmatrix}, \]
which agrees with ([68]). We notice that this discussion remains valid if \( \Omega_n \) admits a potential only locally, as it happens generically for magnetic Bloch bands.

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