GEOMETRIC CURRENTS IN PIEZOELECTRICITY

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Abstract. As a simple model for piezoelectricity we consider a gas of infinitely many non-interacting electrons subject to a slowly time-dependent periodic potential. We show that in the adiabatic limit the macroscopic current is determined by the geometry of the Bloch bundle. As a consequence we obtain the King-Smith and Vanderbilt formula up to errors smaller than any power of the adiabatic parameter.

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1. Introduction

In the year 1880 the brothers Jacques and Pierre Curie discovered that some crystalline solids (like quartz, tourmaline, topaz, ...) exhibit a relevant macroscopic property: if the sample is strained along a particular axis (called the piezoelectric axis) a macroscopic polarization at the edges of the sample appears.

Even though first technological applications already appeared only a few years later, a microscopic understanding of the phenomenon waited many decades after the appearance of quantum mechanics. Up to the mid seventies, it was common lore that the macroscopic (relative) polarization $\Delta\,\mathbf{P} = \mathbf{P}_{\mathrm{fin}} - \mathbf{P}_{\mathrm{in}}$ (*i.e.* the polarization in the final state with respect to the initial state of the sample) was due to the fact that, by deforming the crystal, the fundamental unit cell acquires a *non-vanishing electric dipole moment* with respect to the unperturbed state. As pointed out by Martin in 1974 [10], the previous approach was intrinsically incorrect, since the total polarization should take into account not only the sum of the dipole moments of the unit cells, but also the *transfer of charge* between unit cells. While in the ionic contribution $\Delta\,\mathbf{P}_{\mathrm{ion}}$ the transfer of charge is negligible, it cannot be neglected as far as the electronic contribution $\Delta\,\mathbf{P}_{\mathrm{el}}$ is concerned.[1] It has thus been suggested by Resta [18] to shift the attention from the charge distribution (*i.e.* the electric dipole moment) to the current, *cf.*

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[1] Thereby one clearly assumes that an approximate splitting $\Delta\,\mathbf{P} = \Delta\,\mathbf{P}_{\mathrm{ion}} + \Delta\,\mathbf{P}_{\mathrm{el}}$ is justified.

the review papers [19, 21] and references given therein. In other words one considers

$$\Delta\,\mathbf{P}_{\mathrm{el}} = \int_{T_{\mathrm{in}}}^{T_{\mathrm{fin}}} \mathrm{d}t\ \dot{\mathbf{P}}(t),$$

where $\dot{\mathbf{P}}(t)$, called the *piezoelectric current*, is the real quantity of interest, see equation (1.4) below for the precise definition. Within this framework, Resta used linear response theory in order to conveniently re-express $\Delta\mathbf{P}_{\mathrm{el}}$ in terms of the Bloch functions [18, 19].

Elaborating on Resta's result, King-Smith and Vanderbilt [7] were able to relate the relative polarization to the Berry connection, through the formula

$$\Delta\,\mathbf{P}_{\mathrm{el}} = \frac{1}{(2\pi)^d} \sum_{m=0}^{M} \int_{\mathbb{T}^*} \mathrm{d}k\ \big(\mathcal{A}_m(k,T) - \mathcal{A}_m(k,0)\big), \tag{1.1}$$

where the sum runs over all the occupied Bloch bands, d is the space dimension, $\mathbb{T}^*$ denotes the first Brillouin zone, and $\mathcal{A}_m(k,t)$ is the Berry connection for the mth Bloch band at time $t \in \mathbb{R}$. Thereby the deformation is supposed to take place during the time-interval $I = [0,T]$. The advantage of formula (1.1) is twofold: it depends only on the occupied bands, and it relates the macroscopic polarization to a geometric quantity, which, as discussed later, does not depend on the particular gauge, *i.e.* the choice of the phase of the Bloch functions.

In this paper we provide a rigorous formula for $\Delta\,\mathbf{P}_{\mathrm{el}}$, which is more general than (1.1), by exploiting the fact that the deformation of the crystal is an adiabatic phenomenon, *i.e.* it is extremely slow when measured on the atomic time-scale. Moreover, we provide an alternative derivation of (1.1) relying on the semiclassical dynamics of a state which is essentially concentrated on a single isolated Bloch band.

1.1. **Description of the model.** In the following we shall focus only on the current induced by the electrons, which moreover are assumed to be non-interacting. Thus $\Delta\mathbf{P}_{\mathrm{el}} \equiv \Delta\mathbf{P}$ to simplify the notation. Further we shall restrict ourselves to the *zero temperature regime*, thus taking into account only electrons with an energy below the *Fermi level* E_*.

The physical strain on the lattice will be modeled by a simple *time-dependent Hamiltonian* $H(t)$, to be specified below. Here t is interpreted as the *macroscopic* time-scale which relates to the *microscopic* time s via $t = \varepsilon s$, with $0 < \varepsilon \ll 1$. In other words, a dimensionless small parameter $\varepsilon \ll 1$ is introduced, describing the effects of the mechanical strain as slow variations on the microscopic time scales. Thus we consider the asymptotic behavior as $\varepsilon \to 0$ of the following Schrödinger evolution system

$$\begin{cases} \mathrm{i}\,\varepsilon \dfrac{\mathrm{d}}{\mathrm{d}t} U^\varepsilon(t,0) = H(t)\,U^\varepsilon(t,0), \\ \qquad U^\varepsilon(0,0) = \mathbf{1}_{\mathcal{H}}, \end{cases} \tag{1.2}$$

which consequently describes the dynamics of electrons on the macroscopic time scale $t = \varepsilon s$. For sake of a simpler notation, we shall from now on write $U^\varepsilon(t)$ for $U^\varepsilon(t, 0)$.

Within this setting, the macroscopic polarization $\Delta\mathbf{P}^\varepsilon$ is then defined as follows. The current operator (with respect to *macroscopic* time) is

$$J^\varepsilon := \frac{\mathrm{i}}{\varepsilon}\,[H(t), x]. \tag{1.3}$$

In particular, in the case $H(t) = -\frac{1}{2}\Delta + V_\Gamma(t)$ considered below, one has $J^\varepsilon = -\frac{\mathrm{i}}{\varepsilon}\nabla_x$. Here, and in the following all physical constants are set equal to 1 for convenience. We also assume that the deformation of the solid takes place in a fixed *macroscopic* time interval $I = [0, T]$, *i.e.* that $\operatorname{supp}\dot H(t) \subseteq I$. The state of the system at time t is given by $\rho^\varepsilon(t) := U^\varepsilon(t)\,\rho(0)\,U^\varepsilon(t)^*$, where $\rho(0) := \mathbf{1}_{(-\infty, E_*]}\,(H(0))$ denotes the spectral projection of $H(0)$ below a certain energy E_*, the Fermi energy. The macroscopic piezoelectric current is thus defined as

$$\dot{\mathbf{P}}^\varepsilon(t) := \mathcal{T}(\rho^\varepsilon(t)\,J^\varepsilon). \tag{1.4}$$

where $\mathcal{T}(A)$ denotes the so-called *trace per unit volume* of an operator A, *i.e.*

$$\mathcal{T}(A) := \lim_{n\to\infty} \frac{1}{|\Lambda_n|}\operatorname{Re}\operatorname{Tr}(\mathbf{1}_{\Lambda_n} A)\,, \tag{1.5}$$

and $\mathbf{1}_{\Lambda_n}$ is the characteristic function of a d-dimensional box with finite volume $|\Lambda_n|$, such that $\Lambda_n \nearrow \mathbb{R}^d$. Clearly, the notion of trace per volume is needed since $\rho^\varepsilon(t)$ is not trace class. In summary we get that the macroscopic polarization is given by

$$\Delta\,\mathbf{P}^\varepsilon = \int_0^T \mathrm{d}t\;\mathcal{T}(\rho^\varepsilon(t)\,J^\varepsilon)\,, \tag{1.6}$$

which will be the main object of our investigations.

The previous definitions correspond to the following physical picture. We are considering a large system which, at each fixed macroscopic time, is in thermodynamic equilibrium in the state $\rho(t)$. If $\mu(x)$ is a box, centered at x, whose size is comparable with the lattice spacing, the microscopic current $|\mu(x)|^{-1}\operatorname{Re}\operatorname{Tr}\left(\mathbf{1}_{\mu(x)}\,\rho(t)\,J^\varepsilon\right)$ depends sensitively on the microscopic position x. An average over a larger mesoscopic region Λ_{meso} is needed in order to get rid of the microscopic fluctuations. The use of the thermodynamic limit appearing in (1.4) and (1.6) guaranties that $\dot{\mathbf{P}}^\varepsilon(t)$ and $\Delta\,\mathbf{P}^\varepsilon$ are indeed bulk properties of the system, *i.e.* independent of the actual size and shape of the test volume Λ_{meso}. For a real sample, the charge accumulated during the deformation of the sample at a face Σ is expected to be approximately $\int_\Sigma \Delta\,\mathbf{P}^\varepsilon\cdot n_\Sigma$, where n_Σ is the normal vector to Σ.

Remark 1.1. While we shall discuss the trace per volume in a bit more detail later, let us remark here why (1.5) is the correct definition, at least in the case of the current operator. The current density associated with a Schrödinger wave function $\psi(x)$ is

$$j^\varepsilon(x) := \frac{1}{\varepsilon}\,\mathrm{Im}\,\overline{\psi}(x)\,\nabla\psi(x) = \mathrm{Re}\,\overline{\psi}(x)\,(J^\varepsilon\psi)(x)$$

and thus the current in a region $\Lambda \subset \mathbb{R}^d$ is

$$J^\varepsilon(\Lambda) = \mathrm{Re}\int_\Lambda \mathrm{d}x\,\overline{\psi}(x)\,(J^\varepsilon\psi)(x) = \mathrm{Re}\,\langle \psi, \mathbf{1}_\Lambda J^\varepsilon \psi\rangle\,,$$

which generalizes to $\mathrm{Re}\,\mathrm{Tr}(\mathbf{1}_\Lambda \rho J^\varepsilon)$ for general mixed states ρ and to (1.5) in the thermodynamic limit. One arrives at the same formula by symmetrization of the localized current operator, *i.e.*

$$\mathrm{Re}\,\mathrm{Tr}(\mathbf{1}_\Lambda \rho J^\varepsilon) = \frac{1}{2}\,\mathrm{Tr}(\rho\,(J^\varepsilon \mathbf{1}_\Lambda + \mathbf{1}_\Lambda J^\varepsilon)).$$

Note that one can find other definitions of the current in a volume within the literature, *e.g.* $\mathrm{Tr}(\mathbf{1}_\Lambda \rho J^\varepsilon)$, *i.e.* without taking the real part, or $\mathrm{Tr}(\rho \mathbf{1}_\Lambda J^\varepsilon \mathbf{1}_\Lambda)$, *i.e.* by localizing the current operator through $\mathbf{1}_\Lambda J^\varepsilon \mathbf{1}_\Lambda$. All these definitions yield (presumably) the same thermodynamic limit and thus the same macroscopic current.

To describe the effects of strain upon the solid we consider the standard model in the study of polarization effects, see *e.g.* [7] and [18], namely the following time-dependent Hamiltonian on $\mathcal{H} = L^2(\mathbb{R}^d)$

$$H(t) := -\frac{1}{2}\Delta + V_\Gamma(x,t). \tag{1.7}$$

Since we aim to describe a crystalline structure, the potential $V_\Gamma(x,t)$ in (1.7) is assumed to be *periodic*, for all $t \in I$, w.r.t. to some *regular lattice*[2,3] $\Gamma \simeq \mathbb{Z}^d$, *i.e.*

$$V_\Gamma(x+\gamma,t) = V_\Gamma(x,t), \quad \forall\, x \in \mathbb{R}^d, \gamma \in \Gamma,\ t \in I. \tag{1.8}$$

The centered *fundamental domain* of Γ is

$$Y := \left\{ x \in \mathbb{R}^d :\ x = \sum_{l=1}^d \zeta_l\,\gamma_l,\ \zeta_l \in \left[-\tfrac{1}{2}, \tfrac{1}{2}\right] \right\},$$

where $(\gamma_1, \dots, \gamma_d)$ are the generators of Γ. The corresponding *dual lattice* will be denoted by Γ^* with centered fundamental domain Y^*, usually called (first) *Brillouin zone*. Also, we shall use the notation $\mathbb{T}^* = \mathbb{R}^d/\Gamma^*$, *i.e.* the d-dimensional torus induced by Γ^*. In other words $\mathbb{T}^*$ denotes the Brillouin zone Y^* equipped with periodic boundary conditions.

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[2] We say that a set $\Gamma \subset \mathbb{R}^d$ is a *regular lattice* if Γ is a maximal subgroup of the group $(\mathbb{R}^d, +)$. The requirement of a group structure corresponds to the physical idea of composition of translations.

[3] Notice the distinction between the periodicity lattice Γ, which is a lattice in the sense of the previous definition, and the "atomic lattice" representing the positions of the ionic cores, which generally is not.

A model with a time-independent lattice might seem unrealistic at first glance. However, many piezoelectric materials, *e.g.* GaAs, exhibit a crystallographic structure in which the "atomic lattice", representing the positions of the ionic cores, consists of two sub-lattices corresponding to the two atomic species. Within a good approximation, the deformation of the sub-lattices due to the external strain can be neglected, and the only relevant effect of the strain is a relative displacement of the two sub-lattices [7]. This situation is mathematically described by the model analyzed in this paper, *i.e.* by a time-independent periodicity lattice Γ (fixed with respect to one of the two atomic sub-lattices) and a time-dependent potential, which represents the change of the potential due to the displacement of the other sub-lattice.

1.2. **Synopsis.** Within the framework described above we provide in Theorem 2.3 a rigorous justification and generalization of the King-Smith and Vanderbilt formula (1.1). We show, in particular, that if V_Γ is C^{N+1}, as a map from $I=[0,T]$ to $\mathcal{B}(H^2(\mathbb{R}^d),L^2(\mathbb{R}^d))$, then

$$\Delta\,\mathbf{P}^\varepsilon = -\frac{1}{(2\pi)^d}\int_0^T \mathrm{d}t \int_{\mathbb{T}^*}\mathrm{d}k\ \Theta(k,t) + \mathcal{O}(\varepsilon^N)\,, \tag{1.9}$$

where

$$\Theta(k,t) := -\mathrm{i}\ \mathrm{tr}\left(P(k,t)\left[\partial_t P(k,t),\ \nabla_k P(k,t)\right]\right)\,, \tag{1.10}$$

and $P(k,t)$ is the Bloch-Floquet fiber decomposition[4] of the spectral projector $P(t)=\mathbf{1}_{(-\infty,E(t)]}\left(H(t)\right)$ (the definition of $E(t)$ is given in Assumption 2.2). Here and in the following the symbol tr denotes the trace in the fiber Hilbert space, namely $L^2(Y)$, see Section 3.1. Whenever all Bloch bands within $\mathrm{Ran}\,P(k,t)$ are isolated, formula (1.9) implies (1.1), up to an an error of order $\mathcal{O}(\varepsilon^N)$. Note however that (1.9) is more general, since it can be applied also to situations where band crossings occur. One key ingredient in the rigorous derivation of (1.9) is the super-adiabatic expansion of the fiber decomposition of the time-evolved Fermi projector $\rho^\varepsilon(k,t)$. For fixed $k\in\mathbb{T}^*$ we use the standard super-adiabatic expansion developed by Nenciu [13]. However, since we need to differentiate with respect to k, as suggested by formula (1.10), the expansion needs to be done uniformly on spaces of equivariant functions.

In addition to (1.9), we also provide a dynamical understanding of the same formula based on first order corrections to the semiclassical model of solids. This comes at the price of restricting ourselves to the situation without band crossings. In Theorem 2.4 below we show that the semiclassical equations of motion for an electron in the mth Bloch band, including $\mathcal{O}(\varepsilon)$ corrections, are

$$\begin{cases} \dot q = \nabla_k E_m(k,t) - \varepsilon\,\Theta_m(k,t), \\ \dot k = 0, \end{cases} \tag{1.11}$$

[4] A brief summary of Bloch-Floquet theory is provided in Section 3.1.

with q being the macroscopic position and k the crystal-momentum of the electron. Here Θ_m admits the representation

$$\Theta_m(k,t) = -\partial_t \mathcal{A}_m(k,t) - \nabla_k \phi_m(k,t), \tag{1.12}$$

where one introduces the geometric vector potential (Berry connection)

$$\mathcal{A}_m(k,t) = \mathrm{i} \left\langle \varphi_m(k,t), \nabla_k \varphi_m(k,t) \right\rangle_{L^2(Y)}, \tag{1.13}$$

and the geometric scalar potential

$$\phi_m(k,t) = -\mathrm{i} \left\langle \varphi_m(k,t), \partial_t \varphi_m(k,t) \right\rangle_{L^2(Y)}, \tag{1.14}$$

with φ_m being the mth Bloch eigenfunction. As suggested by the previous formulae, the vector field Θ_m exhibit an interesting analogy with the electric field. Moreover both Θ and Θ_m correspond to the curvature of a connection on a bundle over $\mathbb{T}^* \times \mathbb{R}$, *cf.* Section 6 for a broader discussion on this. It is then natural to baptize Θ the *piezoelectric curvature.*

As shown in Section 2, the King-Smith and Vanderbilt formula (1.1) follows from the corrected semiclassical equations of motion (1.11) by a straightforward classical statistical mechanics argument. Indeed, it a standard textbook argument which shows that the semiclassical model without the $\mathcal{O}(\varepsilon)$ corrections implies that filled band do not contribute to the current at all.

Remark 1.2. There is a related result by Elgart and Schlein [3] who derive the adiabatic charge transport for a class of Landau type Hamiltonians. They also rely on Nenciu's super-adiabatic approximation to the time evolved Fermi projector. Here we only remark that there are important differences between our result and [3]. Details are given in the remarks after the statement of Theorem 2.3.

Our methods also apply to the case of a periodic deformation of the crystal, *i.e.* $H(t+T) = H(t)$ for every $t \in \mathbb{R}$. In such case, formula (1.9) implies that $\Delta \mathbf{P}^\varepsilon$ is, up to errors of order $\mathcal{O}(\varepsilon^N)$, an integer multiple of a fundamental quantity, in agreement with a previous observation by Thouless [26]. Further analysis is required to show that $\Delta \mathbf{P}^\varepsilon$ is actually nonzero in a specific model, as done in [1] for the case of Harper-like models. In general, in order to obtain a nonzero polarization one has to choose a map $t \mapsto H(t)$ that, in a suitable space $\mathcal{M}$ of hamiltonian operators, describes a loop around a manifold $\mathcal{M}_{\mathrm{cr}} \subset \mathcal{M}$ consisting of hamiltonian operators for which the gap assumption (Assumption 2.2) is violated. This fact is crucially used in [1], while an analogous situation has been investigated in the context of molecular physics [4].

The paper is now organized as follows. The precise assumptions and the main mathematical results are stated in Section 2. In Section 3 we collect some preliminary results used in the following. In Section 4 we present the so-called super-adiabatic theorem, which comprises the main mathematical step towards our final results, to be proved in Section 5. In Section 6 we discuss in more detail the geometrical interpretation of our results.

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2. Main results

The basic assumption on the potential V_Γ will be as follows.

Assumption 2.1. *For all $t \in \mathbb{R}$ the potential $V_\Gamma(t)$ is H_0-bounded with relative bound smaller than 1. We assume that*

$$V_\Gamma \in C^{N+1}(\mathbb{R}, \mathcal{B}(H^2(\mathbb{R}^d), L^2(\mathbb{R}^d)))$$

for some $N \in \mathbb{N}$, and that $\dot{V}_\Gamma(t)$ is compactly supported in a bounded interval $I = [0, T]$ and $H(t)$-form bounded for all $t \in I$.

From this assumption it follows in particular that $H(t)$ is self-adjoint on the Sobolev space $H^2(\mathbb{R}^d)$, for all $t \in I$. Moreover this implies the existence of a unique unitary propagator $U^\varepsilon(t)$ obeying (1.2).

From now on we impose the following condition on the spectrum of $H(t)$:

Assumption 2.2. *There exists a continuous function $E(t)$, such that $E(0) = E_*$, which satisfies*

$$\operatorname{dist}(E(t), \sigma(H(t))) > 0, \quad \textit{for all } t \in I.$$

It is not assumed, however, that there is an energy E_*, independent of time, which lies in a spectral gap for all $t \in I$, *i.e.* the gap might move up and down in energy.

Theorem 2.3. *Let Assumption 2.1 hold and let $P(k,t)$ be the Bloch-Floquet representation of the spectral projector $P(t) = \mathbf{1}_{(-\infty, E(t)]}(H(t))$, where $E(t)$ is as in Assumption 2.2. Then there exists an orthogonal projector $P_N^\varepsilon(k,t)$ with*

$$\|P(k,t) - P_N^\varepsilon(k,t)\| = \mathcal{O}(\varepsilon)\,,$$

such that the macroscopic current can be expressed as

$$\begin{aligned} \mathcal{T}(\rho^\varepsilon(t)\, J^\varepsilon) &= -\frac{1}{(2\pi)^d}\int_{\mathbb{T}^*} \mathrm{d}k\, \Theta_N^\varepsilon(k,t) + \mathcal{O}(\varepsilon^N) \\ &= -\frac{1}{(2\pi)^d}\int_{\mathbb{T}^*} \mathrm{d}k\, \Theta(k,t) + \mathcal{O}(\varepsilon)\,, \end{aligned} \tag{2.1}$$

where $\Theta(k,t)$ is given by (1.10) and $\Theta_N^\varepsilon(k,t)$ is

$$\Theta_N^\varepsilon(k,t) := -\mathrm{i}\ \mathrm{tr}\left(P_N^\varepsilon(k,t)\,[\partial_t P_N^\varepsilon(k,t),\ \nabla_k P_N^\varepsilon(k,t)\,]\,\right). \tag{2.2}$$

The total transported charge is then

$$\Delta\mathbf{P}^\varepsilon := \int_0^T \mathrm{d}t\ \mathcal{T}(\rho^\varepsilon(t)\, J^\varepsilon) = -\frac{1}{(2\pi)^d}\int_0^T \mathrm{d}t \int_{\mathbb{T}^*} \mathrm{d}k\, \Theta(k,t) + \mathcal{O}(\varepsilon^N)\,. \tag{2.3}$$

Remarks

(1) Note that the error estimate in (2.3) is better than what one would naively guess from (2.1). As mentioned before, the King-Smith and Vanderbilt formula (1.1) was originally derived using linear response theory. Our result (2.3) confirms the rule that there are no power law corrections to Kubo's formula, see also [8].

(2) Note that $\Theta(k,t)$ is well defined *independently* of whether there are energy level crossings within the occupied Bloch bands, *i.e.* within $\operatorname{Ran} P(k,t)$, or not, and independently of whether the complex vector bundle defined by $\operatorname{Ran} P(k,t)$, for fixed $t \in I$, is trivial or not.

(3) From the physical point of view, Assumption 2.2 corresponds to the requirement that the solid remains an insulator during the adiabatic deformation of the crystal, a condition verified in the experiments. Mathematically one could relax Assumption 2.2 to hold only locally on the first Brillouin zone. More precisely, Theorem 2.3 is still valid by the same proof, if there exist a continuous function $E(k,t)$, such that $E(k,0) = E_*(k)$, which satisfies

$$\operatorname{dist}(E(k,t), \sigma(H(k,t))) > 0, \quad \text{for all } t \in I \text{ and } k \in \mathbb{T}^*.$$

(4) As remarked before, our result looks and to some extent is similar to the derivation of Kubo's formula for Landau type Hamiltonians by Elgart and Schlein [3]. Therefore we would like to explicitly point out some crucial differences. In [3] only the leading order expression for the current is computed. While it can be seen from (2.3) that the leading order expression for the total charge is valid up to errors of order ε^{N+1}, this is not true for the current itself, which is as well an observable quantity. Another difference is that we are looking at a bulk property, the macroscopic current, while in [3] the authors consider the current induced in a fixed finite region. On the other hand, since we heavily use the periodicity of the problem, we can't allow for small but non-periodic perturbations of the Hamiltonian so easily, as is done in [3].

If all Bloch bands within $\operatorname{Ran} P(k,t)$ are isolated, then $\Theta(k,t)$ can be decomposed as

$$\Theta(k,t) = \sum_{m=0}^{M} \Theta_m(k,t), \qquad M = \dim\left(\operatorname{Ran} P(k,t)\right), \tag{2.4}$$

where Θ_m admits the representation (1.12). In particular (2.4), together with (2.3), gives

$$\Delta\, \mathbf{P}^\varepsilon = \frac{1}{(2\pi)^d} \sum_{m=0}^{M} \int_{\mathbb{T}^*} \mathrm{d}k \, \big(\mathcal{A}_m(k,T) - \mathcal{A}_m(k,0)\big) + \mathcal{O}(\varepsilon^{N+1}), \tag{2.5}$$

where the contribution of $\phi_m(k,t)$ vanishes due to periodicity, thus yielding a rigorous justification of the King-Smith and Vanderbilt formula (1.1).

In our second result we give an alternative derivation of the King-Smith and Vanderbilt formula based on first order corrections to the the semiclassical model in solids. To this end we restrict ourselves to the case of a simple isolated Bloch band $E_m(\cdot,t)$, with the corresponding eigenprojector denoted as $P_m(\cdot,t)$. For sake of a simple discussion, we consider pure state solutions to the Schrödinger equation,

$$\psi^\varepsilon(t,x) = U^\varepsilon(t)\,\psi_0(x), \quad \psi_0 \in \operatorname{Ran} P_m(0), \tag{2.6}$$

where the unitary propagator $U^\varepsilon(t)$ solves (1.2). However the result extends without major difficulties to the case of a mixed state, provided it is initially concentrated on the m-th Bloch band, *i.e.* $\rho_0 = P_m(0)\rho_0 P_m(0)$.

Since we are interested in the macroscopic charge distribution only, we study the corresponding *macroscopic Wigner function* defined as

$$w[\psi^\varepsilon(t)](q,k) := \frac{1}{(2\pi\varepsilon)^d}\int_{\mathbb{R}^d} \mathrm{d}\eta\, \overline{\psi^\varepsilon}\left(t, \frac{q}{\varepsilon}+\frac{\eta}{2}\right)\psi^\varepsilon\left(t,\frac{q}{\varepsilon}-\frac{\eta}{2}\right)\mathrm{e}^{\mathrm{i}\eta\cdot k}. \tag{2.7}$$

The variable $q := \varepsilon x$ will be called the macroscopic position and $k \in \mathbb{R}^d$. The Wigner function is the quantum mechanical analogue of the phase space distribution in classical statistical mechanics, even though $w[\psi^\varepsilon(t)]$ is not positive in general (for more details on Wigner functions we refer to [5]). Since the natural phase space in our case is $\mathbb{R}^d\times\mathbb{T}^*$ rather than $\mathbb{R}^d\times\mathbb{R}^d$, we fold the Wigner function onto $\mathbb{R}^d\times\mathbb{T}^*$ and use the *reduced Wigner function* [24] given by

$$w_{\mathrm{r}}[\psi^\varepsilon(t)](q,k) = \sum_{\gamma^*\in\Gamma^*} w[\psi^\varepsilon(t)](q,k+\gamma^*). \tag{2.8}$$

The main use of $w_{\mathrm{r}}[\psi^\varepsilon(t)]$ is that it allows to compute expectation values of *Weyl quantized operators* $a^W(\varepsilon x, -\mathrm{i}\nabla_x)$, *cf.* [5, 23] with semiclassical symbols $a \in C_{\mathrm{b}}^\infty(\mathbb{R}^6)$, such that $a(q,k+\gamma^*) = a(q,k)$ for all $\gamma^*\in\Gamma^*$, via the following formula

$$\left\langle \psi^\varepsilon(t), a^W\,\psi^\varepsilon(t)\right\rangle_{L^2(\mathbb{R}^d)} = \iint_{\mathbb{R}^d\times\mathbb{T}^*}\mathrm{d}q\,\mathrm{d}k\; a(q,k)\,w_{\mathrm{r}}[\psi^\varepsilon(t)](q,k)\,. \tag{2.9}$$

Above, C_{b}^∞ denotes the space of smooth functions which are bounded together with all their partial derivatives.

The following theorem states that the Wigner function of the solution to the Schrödinger equation can be approximately obtained by transporting the Wigner function of the initial datum along the flow lines of a classical flow on $\mathbb{R}^d\times\mathbb{T}^d$, the so called semiclassical model, *cf.* (2.10).

Theorem 2.4. *Let the potential V_Γ satisfy Assumption 2.1 with $N=1$. Also let $E_m(k,t)$ be an isolated, non-degenerated Bloch band for all $t\in I$ and denote by $P_m(t)$ the corresponding eigenprojector. Then, for any semiclassical observable a^W, corresponding to a symbol $a\in C_{\mathrm{b}}^\infty(\mathbb{R}^{2d})$ such that $a(x,k+\gamma^*) = a(x,k)$ for all $\gamma^*\in\Gamma^*$, there is a constant C_a such that for any $\psi_0\in\operatorname{Ran}P_m(0)$ and it holds*

$$\left|\iint_{\mathbb{R}^d\times\mathbb{T}^*}\mathrm{d}q\,\mathrm{d}k\; a(q,k)\big(w_{\mathrm{r}}[\psi^\varepsilon(t)] - w_{\mathrm{r}}[\psi_0]\circ\Phi_m^\varepsilon(0,t)\big)(q,k)\right| \le \varepsilon^2 C_a\,|t|(1+|t|),$$

where $\Phi^\varepsilon_m(t,0) : \mathbb{R}^6 \to \mathbb{R}^6$ denotes the ε-corrected semiclassical flow in the mth Bloch band, given by the solution flow of

$$\begin{cases} \dot q = \nabla_k E_m(k,t) - \varepsilon\, \Theta_m(k,t), \\ \dot k = 0. \end{cases} \tag{2.10}$$

In (2.10) one interprets $q(t)$ as the macroscopic position and $k(t)$ as the crystal-momentum of the electron.

The semiclassical equations of motion (2.10) can now be taken as a starting point for a classical statistical mechanics analysis of transport properties, *cf.* [27]. Although the equations of motion (2.10) are non-autonomous, they still allow for a stationary measure. The stationary measure for a filled band at zero temperature and with density of one particle per unit cell is equi-distribution on phase space $\mathbb{R}^d \times \mathbb{T}^*$ with density $(|Y||Y^*|)^{-1} = (2\pi)^{-d}$. The macroscopic current at time $t \in I$ contributed from such a filled band is then

$$\begin{aligned} j^\varepsilon_m(t) &= \frac{1}{\varepsilon(2\pi)^d} \int_{\mathbb{T}^*} \mathrm{d}k\, \dot q(k,t) \\ &= \frac{1}{\varepsilon(2\pi)^d} \int_{\mathbb{T}^*} \mathrm{d}k\, (\nabla_k E_m(k,t) - \varepsilon\, \Theta_m(k,t)) \\ &= -\frac{1}{(2\pi)^d} \int_{\mathbb{T}^*} \mathrm{d}k\, \Theta_m(k,t)\,. \end{aligned}$$

Integration over the relevant time interval and summation over all filled bands yields again the correct formula (2.3) for the polarization. Hence one can understand the piezoelectric current even quantitatively on the basis of the semiclassical model if one takes into account first order corrections. The situation is similar to the quantum Hall current, *cf.* [14, 16].

3. Technical preliminaries

To obtain a more detailed description of the properties of $H(t)$, we shall extensively use the well known *Bloch-Floquet theory*, some basic facts of which will be recapitulated in the next subsection. More precisely, we will use a variant of the Bloch-Floquet transform which is sometimes called the Zak tranform [29]. A comparison of the two definitions is given in [16].

3.1. **The Bloch-Floquet representation and the trace per volume.**

One exploits the periodicity of the problem in order to separate the dynamics at the microscopic scale from the long range dynamics. Denoting by $\mathbb{T}^d \equiv \mathbb{R}^d/\Gamma$ the d-dimensional torus (corresponding to the fundamental cell Y equipped with periodic boundary conditions), the Bloch-Floquet-Zak transform

$$\mathcal{Z} : L^2(\mathbb{R}^d_x) \cong L^2(\Gamma \times Y) \cong \ell^2(\Gamma) \otimes L^2(Y) \to L^2(Y^*_k, |Y^*|^{-1}\mathrm{d}k) \otimes L^2(\mathbb{T}^d_y)$$

is just the regular Fourier transform $\mathcal{F}$ on the factor $\ell^2(\Gamma)$ followed by a multiplication with $\exp(-\mathrm{i}y\cdot k)$, *i.e.*

$$(\mathcal{Z}\psi)(k,y)=\mathrm{e}^{-\mathrm{i}y\cdot k}(\mathcal{F}\otimes\mathbf{1}\psi)(k,y)=\sum_{\gamma\in\Gamma}\mathrm{e}^{-i(y+\gamma)\cdot k}\psi(y+\gamma),$$

for $k\in Y^*, y\in\mathbb{R}^d$. One immediately gets the following periodicity properties

$$\begin{aligned}(\mathcal{Z}\psi)(k,y+\gamma)&=(\mathcal{Z}\psi)(k,y),\quad\forall\gamma\in\Gamma,\\(\mathcal{Z}\psi)(k+\gamma^*,y)&=\mathrm{e}^{-\mathrm{i}y\cdot\gamma^*}(\mathcal{Z}\psi)(k,y),\quad\forall\gamma^*\in\Gamma^*.\end{aligned}\tag{3.1}$$

The second line in (3.1) induces a unitary representation of the group of lattice translations in Γ^*, given by

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

where $\tau(\gamma^*)$ acts as the multiplication operator by $\exp(-\mathrm{i}y\cdot\gamma^*)$ on $L^2(\mathbb{T}^d_y)$. Next, one easily checks that

$$\begin{aligned}\mathcal{Z}(-\mathrm{i}\nabla_x)\mathcal{Z}^{-1}&=\mathbf{1}\otimes(-\mathrm{i}\nabla_y)+k\otimes\mathbf{1},\\\mathcal{Z}x\mathcal{Z}^{-1}&=\mathrm{i}\nabla_k^\tau.\end{aligned}$$

Here the operator $-\mathrm{i}\nabla_y$ acts on the domain $\mathcal{D}_1\equiv H^1(\mathbb{T}^d_y)$, *i.e.* is equipped with periodic boundary conditions. On the other hand the domain of $\mathrm{i}\nabla_k^\tau$ is the space of distributions in $H^1(\mathbb{R}^d,L^2(\mathbb{T}^d_y))$ which satisfy the y-dependent (quasi-periodic) boundary conditions associated with the second line in (3.1).

It is well known that the Bloch-Floquet transformation of $H(t)$, defined in (1.7), yields the fibered operator

$$\mathcal{Z}H(t)\mathcal{Z}^{-1}=\int_{Y^*}^{\oplus}\mathrm{d}k\,H(k,t)$$

where

$$H(k,t):=\frac{1}{2}(-\mathrm{i}\nabla_y+k)^2+V_\Gamma(y,t),\quad k\in Y^*,\tag{3.2}$$

with corresponding domain $\mathcal{D}_2\equiv H^2(\mathbb{T}^d_y)$, provided Assumption 2.1. The spectrum of $H(k,t)$ is pure point and intensively studied for example in [28]. The so called *Bloch bands* $E_m(k,t)$, $m\in\mathbb{N}$, and the *Bloch projectors* $P_m(k,t)$, are consequently defined to be eigenvalues and corresponding spectral projectors of $H(k,t)$, *i.e.*

$$H(k,t)P_m(k,t)=E_m(k,t)P_m(k,t),\quad m\in\mathbb{N}.$$

Thereby, for definiteness, the eigenvalues $\{E_m\}_{m\in\mathbb{N}}$ are enumerated, according to $E_0(k,t)\leq E_1(k,t)\leq\dots$. The corresponding (normalized) *eigenfunctions* $\{\varphi_m(k,t)\}_{m\in\mathbb{N}}\subset\mathcal{D}_2$ are called *Bloch functions*. For any fixed $k\in Y^*$, $t\in I$, they form an orthonormal basis of $L^2(\mathbb{T}^d_y)$.

The *extended Bloch bundle* is, by definition, the sub-bundle of the trivial bundle

$$(Y^*_k\times\mathbb{R}_t)\times L^2(\mathbb{T}^d_y)\tag{3.3}$$

whose fiber at the point (k,t) is the range of the orthogonal projector $P_m(k,t)$, see [17] for a broader discussion.

Remark 3.1. (Definition of the extended Bloch bundle) More formally, the extended Bloch bundle ξ is defined in the following way. First one introduces on the set $\mathbb{R}^d \times \mathbb{R} \times \mathcal{H}_{\mathrm{f}}$ the equivalence relation $\sim_\tau$, where

$$(k,t,\varphi) \sim_\tau (k',t',\varphi') \quad \Leftrightarrow \quad (k',t',\varphi') = (k+\lambda\,, t,\, \tau(\lambda)\varphi) \quad \text{for some } \lambda \in \Gamma^*.$$

The equivalence class with representative (k,t,φ) is denoted as $[k,t,\varphi]$. Then the total space E of the bundle ϑ is defined as

$$E := \Big\{ [k,t,\varphi] \in (\mathbb{R}^d \times \mathbb{R} \times \mathcal{H}_{\mathrm{f}})/\!\sim_\tau : \quad \varphi \in \operatorname{Ran} P_m(k,t) \Big\}.$$

This definition does not depend on the representative in view of the covariance property (3.1). The base space is the cylinder $B = \mathbb{T}^* \times \mathbb{R}$, where $\mathbb{T}^* := \mathbb{R}^d/\Gamma^*$, and the projection to the base space $\pi : E \to B$ is $\pi[k,t,\varphi] = (\mu(k),t)$, where μ is the projection modulo Γ^*, $\mu : \mathbb{R}^d \to \mathbb{T}^*$. One checks that $\xi = (E \xrightarrow{\pi} B)$ is a smooth complex line bundle.

Clearly, if one considers the projector $P(k,t)$ corresponding to a family of Bloch bands, the same procedure define a complex vector bundle over B, with typical fiber $\mathbb{C}^r$, $r = \dim \operatorname{Ran} P(k,t)$. We will use the same notation and terminology for the two previous cases, the difference being clear from the context.

In Bloch-Floquet representation the projector $P(t) = \mathbf{1}_{(-\infty,E(t)]}H(t)$ is again a fibered operator, in the following denoted by $P(k,t)$, and $\operatorname{Ran} P(k,t)$ has constant dimension $M \in \mathbb{N}$. Assumption 2.2 then implies that the lowest M Bloch bands are separated from the other bands by a finite gap. We therefore call them *isolated*.

Remark 3.2. In terms of Bloch functions we have

$$P(k,t) = \sum_{m=0}^{M} |\varphi_m(k,t)\rangle\langle\varphi_m(k,t)|.$$

However, whereas $\varphi_m(k,t)$ may not be a smooth function of k in general, due to band crossings, the operator $P(k,t)$ indeed is a smooth functions of k due to Assumption 2.2.

Finally let us state the following auxiliary result, to be used later on.

Lemma 3.3. *Let A be a bounded operator acting on $L^2(\mathbb{R}^d)$ which is fibered in Bloch-Floquet representation, i.e.*

$$\mathcal{Z} A \mathcal{Z}^{-1} = \int_{\mathbb{T}^*}^{\oplus} \mathrm{d}k\, A(k)\,.$$

If, in addition, $A(k) \in \mathcal{B}(L^2(\mathbb{T}^d_y))$ is trace class, with $\operatorname{tr}|A(k)| < C$, for all $k \in \mathbb{T}^*$, then the trace per unit cell of A exists and is given by

$$\operatorname{Tr}(A\,\mathbf{1}_{Y_\lambda}) = \frac{1}{|Y^*|}\int_{\mathbb{T}^*} \mathrm{d}k\, \operatorname{tr} A(k)\,, \tag{3.4}$$

where $Y_\lambda \subset \mathbb{R}^d$ with $\lambda \in \mathbb{R}^d$ denotes any translate of the fundamental domain Y of the lattice Γ and $\mathbf{1}_{Y_\lambda}(x)$ is the characteristic function on Y_λ. Moreover

$$\mathcal{T}(A) := \lim_{n\to\infty} \frac{1}{|\Lambda_n|} \operatorname{Re} \operatorname{Tr}(A\,\mathbf{1}_{\Lambda_n}) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^*} \mathrm{d}k \, \operatorname{Re} \operatorname{tr} A(k)\,.$$

Proof. For $\lambda \in \Gamma$, let $Y_\lambda = Y + \lambda$ be an arbitrary, but fixed, Γ-translate of the unit cell Y of Γ. Having in mind that A is fibered, thus $A = \mathscr{T}_\lambda{}^* \, A \, \mathscr{T}_\lambda$, with $\mathscr{T}_\lambda$ denoting the lattice translation by $\lambda \in \Gamma$, we immediately get that

$$\operatorname{Tr}(A\mathbf{1}_Y) = \operatorname{Tr}(A \, \mathscr{T}_\lambda \, \mathbf{1}_Y \, \mathscr{T}_\lambda{}^*) = \operatorname{Tr}(A\,\mathbf{1}_{Y_\lambda}).$$

In order to evaluate the trace $\operatorname{Tr}(A\,\mathbf{1}_Y)$, we define the following orthonormal basis of $\operatorname{Ran} \mathbf{1}_Y \subset L^2(\mathbb{R}^d)$. Let

$$g_{\gamma^*}(x) := \mathbf{1}_Y(x)\, \mathrm{e}^{\mathrm{i}\gamma^*\cdot x} \quad \text{for } \gamma^* \in \Gamma^*\,,$$

then

$$\mathcal{Z} g_{\gamma^*}(k,y) = \mathrm{e}^{-\mathrm{i}y\cdot k} \; \mathrm{e}^{\mathrm{i}\gamma^*\cdot y} = e_{\gamma^*}(y)\,,$$

where for fixed $k \in \mathbb{T}^*$ the family of functions $e_{\gamma^*}(y) := \mathrm{e}^{\mathrm{i}(\gamma^*-k)\cdot y}$, $\gamma^* \in \Gamma^*$, form an orthonormal basis of $L^2(\mathbb{T}^d)$. Hence,

$$\begin{aligned}
\operatorname{Tr}(A\,\mathbf{1}_Y) &= \sum_{\gamma^*} \langle g_{\gamma^*},\, A\,\mathbf{1}_Y\, g_{\gamma^*}\rangle \\
&= \frac{1}{|Y^*|} \int_{\mathbb{T}^*} \mathrm{d}k \sum_{\gamma^*} \int_{\mathbb{T}} \mathrm{d}y\, e^*_{\gamma^*}(y)\, A(k)\, e_{\gamma^*}(y) \\
&= \frac{1}{|Y^*|} \int_{\mathbb{T}^*} \mathrm{d}k \sum_{\gamma^*} \langle e_{\gamma^*},\, A(k) e_{\gamma^*}\rangle_{\mathcal{H}_\mathrm{f}} = \frac{1}{|Y^*|} \int_{\mathbb{T}^*} \mathrm{d}k \; \operatorname{tr} A(k)\,.
\end{aligned}$$

For an arbitrary translate $Y + \alpha$ of Y, $\alpha \in \mathbb{R}^d$, exactly the same argument works with the translated basis $g^\alpha_{\gamma^*}(x) := g_{\gamma^*}(x-\alpha)$ resp. $\mathcal{Z} g^\alpha_{\gamma^*}(k,y) = \mathrm{e}^{\mathrm{i}\alpha\cdot k} \; e_{\gamma^*}(y-\alpha)$.

Consequently, for an arbitrary measurable subset $\Lambda \subset Y$ the same computation with $\mathbf{1}_Y$ replaced by $\mathbf{1}_\Lambda$ shows that

$$|\operatorname{Tr}(A\,\mathbf{1}_\Lambda)| \le \frac{1}{|Y^*|} \int_{\mathbb{T}^*} \mathrm{d}k \; \operatorname{tr} |A(k)| \le C\,.$$

From this it follows that for any sequence (Λ_n) of boxes with $\Lambda_n \nearrow \mathbb{R}^d$ one has

$$\mathcal{T}(A) := \lim_{n\to\infty} \frac{1}{|\Lambda_n|} \operatorname{Re} \operatorname{Tr}(A\mathbf{1}_{\Lambda_n}) = \frac{1}{|Y||Y^*|} \int_{\mathbb{T}^*} \mathrm{d}k \operatorname{Re} \operatorname{tr} A(k)\,. \tag{3.5}$$

□

Remark 3.4. As far as the sequence $\Lambda_n \nearrow \mathbb{R}^d$ is concerned, one can replace the sequence of finite volume boxes introduced for the definition of the trace per unit volume by any *Følner sequence*, *i.e.* any sequence of measurable sets whose union adds up to $\mathbb{R}^d$ and such that for any $a \in \mathbb{R}^d$ one has $\lim_{n\to\infty} |(\Lambda_n + a) \setminus \Lambda_n|/|\Lambda_n| = 0$.

3.2. **The concept of equivariance.** In order to make precise statements, we have to introduce some more notations. Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be separable Hilbert spaces and τ_1 and τ_2 be unitary representations of Γ^* on $\mathcal{H}_1$ resp. $\mathcal{H}_2$.

We say that a function $f \in C(\mathbb{R}^d_k, \mathcal{H}_1)$ is τ_1-*equivariant*, if

$$f(k - \gamma^*) = \tau_1(\gamma^*) f(k) \quad \forall\, \gamma^* \in \Gamma^*, k \in \mathbb{R}^d. \tag{3.6}$$

We say that a bounded operator valued function $f \in C(\mathbb{R}^d_k, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ is (τ_1, τ_2)-*equivariant*, if

$$f(k - \gamma^*) = \tau_2(\gamma^*)\, f(k)\, \tau_1(\gamma^*)^{-1} \quad \forall\, \gamma^* \in \Gamma^*, k \in \mathbb{R}^d. \tag{3.7}$$

The space of smooth τ_1- resp. (τ_1, τ_2)-equivariant functions is then denoted by

$$\mathcal{E}_{\mathcal{H}_1} = \{ f \in C^\infty(\mathbb{R}^d_k, \mathcal{H}_1) : \text{relation (3.6) holds} \}$$

resp.

$$\mathcal{E}_{\mathcal{H}_1,\mathcal{H}_2} = \{ f \in C^\infty(\mathbb{R}^d_k, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)) : \text{relation (3.7) holds} \}.$$

The family of seminorms

$$\|f\|_\sigma := \sup_{k \in Y^*} \|\partial^\sigma_k f(k)\|_{\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)}, \quad \sigma \in \mathbb{N}^d_0, \tag{3.8}$$

turns $\mathcal{E}_{\mathcal{H}_1,\mathcal{H}_2}$ into a Frechet space. Here $\mathbb{N}_0 = \{0, 1, 2, \ldots\}$.

In the following there will be only two cases appearing: The unitary representation of Γ^* on $L^2(\mathbb{T}^d)$, or on the domain $\mathcal{D}_2 = H^2(\mathbb{T}^d_y)$, which is given by $\tau(\gamma^*)$, the operator of multiplication with $\exp(\mathrm{i}y \cdot \gamma^*)$. On all other spaces (in particular on $\mathbb{C}^{|M|}$ below) we always use the trivial representation $\tau \equiv \mathbf{1}$. In the latter case equivariant functions are just periodic. Therefore we will just say that a family of operators is *equivariant*, understanding that the representations of Γ^* on the respective spaces are clear from the context.

Each equivariant family $f \in C(\mathbb{R}^d_k, \mathcal{B}(\mathcal{H}_1, \mathcal{H}_2))$ defines an associated operator in $\mathcal{B}(L^2(Y^*, \mathcal{H}_1), L^2(Y^*, \mathcal{H}_2))$ through

$$(f\psi)(k) = f(k)\psi(k) \quad \forall\, k \in Y^*$$

and the norms are related by

$$\|f\|_{\mathcal{B}(L^2(Y^*,\mathcal{H}_1),L^2(Y^*,\mathcal{H}_2))} = \sup_{k \in Y^*} \|f(k)\|_{\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)}\,.$$

An operator in $\mathcal{B}(L^2(Y^*, \mathcal{H}_1), L^2(Y^*, \mathcal{H}_2)) = \mathcal{B}(L^2(Y^*) \otimes \mathcal{H}_1, L^2(Y^*) \otimes \mathcal{H}_2)$ is called equivariant, if it is given by an equivariant family. Note that the composition of two equivariant operators is equivariant.

We will say that $f^\varepsilon \in \mathcal{E}_{\mathcal{H}_1,\mathcal{H}_2}$ *is of order* ε^n *in* $\mathcal{E}_{\mathcal{H}_1,\mathcal{H}_2}$, shortly $\|f^\varepsilon\|_{\mathcal{E}_{\mathcal{H}_1,\mathcal{H}_2}} = \mathcal{O}(\varepsilon^n)$, or $f^\varepsilon = \mathcal{O}_{\mathcal{E}}(\varepsilon^n)$ and thereby abusing the norm-symbol, if for each multi-index $\sigma \in \mathbb{N}^d_0$ there is a constant $C_\sigma < \infty$ such that

$$\|f\|_\sigma < C_\sigma \varepsilon^n\,.$$

In the same spirit, we say that a map $t \mapsto f(t)$ from $I \subset \mathbb{R}$ to $\mathcal{E}_{\mathcal{H}_1,\mathcal{H}_2}$ is differentiable, if it is differentiable with respect to all the seminorms $\|\cdot\|_\sigma$ defined by (3.8).

Proposition 3.5. *Assume that the family of bands* $\{E_m(k,t)\}_{m\in M}$*, M some finite index set, is isolated from the rest of the spectrum for* $(k,t)\in Y^*\times I$ *and denote the corresponding spectral projection by* $P(k,t)$*. Then*

$$(H(\cdot,t)-\mathrm{i})^{-1}\in\mathcal{E}_{L^2(\mathbb{T}^d),\mathcal{D}_2}\quad\textit{and}\quad P(\cdot,t)\in\mathcal{E}_{L^2(\mathbb{T}^d),\mathcal{D}_2}\,,\quad\forall\, t\in I.$$

Moreover if $(H(k,\cdot)-\mathrm{i})^{-1}\in C^{N+1}(I,\mathcal{B}(L^2(\mathbb{T}^d),\mathcal{D}_2))$ *for all* $k\in Y^*$ *then*

$$(H(\cdot,\cdot)-\mathrm{i})^{-1}\in C^{N+1}(I,\mathcal{E}_{L^2(\mathbb{T}^d),\mathcal{D}_2})\quad\textit{and}\quad P(\cdot,\cdot)\in C^{N+1}(I,\mathcal{E}_{L^2(\mathbb{T}^d),\mathcal{D}_2}).$$

Proof. Let $C(t)\subset\varrho\,(H(k,t))\subset\mathbb{C}$ be a cycle encircling $\{E_m(k,t)\}_{m\in M}$ once in the positive sense, but no other part of the spectrum of $H(k,t)$. Then

$$P(k,t)=\frac{\mathrm{i}}{2\pi}\oint_{C(t)}\mathrm{d}z\,(H(k,t)-z)^{-1}\,.$$

Then the statements about $P(k,t)$ follow from the corresponding statements about the resolvent. For $z\in\varrho\,(H(k,t))$ we have

$$\begin{aligned}R_z(k-\gamma^*,t)&=(\tau(\gamma^*)(H(k,t)-z)\tau(\gamma^*)^{-1})^{-1}\\&=\tau(\gamma^*)(H(k,t)-z)^{-1}\tau(\gamma^*)^{-1}\\&=\tau(\gamma^*)R_z(k,t)\tau(\gamma^*)^{-1}\,,\end{aligned}$$

and thus $R_z(\cdot,t)$ is equivariant. The statements about the differentiability follow from

$$\partial_{k_j}R_z(k,t)=-R_z(k,t)\,(\partial_{k_j}H(k,t))\,R_z(k,t)$$

resp.

$$\partial_t R_z(k,t)=-R_z(k,t)\,(\partial_t H(k,t))\,R_z(k,t)$$

and iterations of these formulas. □

For the proof of the super-adiabatic theorem we shall also need the following observation:

Lemma 3.6. *There exists a smooth τ-equivariant orthonormal basis* $(\chi_\alpha(k,t))_{\alpha=1}^M$ *of* $\operatorname{Ran}P(k,t)$ *such that the coefficient of the Berry connection in the time direction vanishes identically in this basis. More precisely, for all* $(t,k)\in I\times Y^*$ *and* $\alpha,\beta\in\{1,\dots,M\}$ *it holds that*

$$\phi_{\alpha\beta}(k,t):=\mathrm{i}\langle\chi_\alpha(k,t),\partial_t\chi_\beta(k,t)\rangle_{L^2(\mathbb{T}^d_y)}\equiv 0\,.$$

If $P(\cdot,\cdot)\in C^{N+1}(I,\mathcal{E}_{L^2(\mathbb{T}^d),\mathcal{D}_2})$*, then* $\chi_\alpha(\cdot,\cdot)\in C^{N+1}(I,\mathcal{E}_{\mathcal{D}_2})$.

Proof. First, we choose at time $t=0$, a smooth and τ-equivariant orthonormal basis $\chi(k,0)=(\chi_1(k,0),\dots,\chi_M(k,0))$ of $\operatorname{Ran}P(k,0)$. We can always find such a basis since the complex vector bundle (over the torus) defined by $P(k,0)$ is trivial. As shown in [17], triviality of the Bloch bundle with M-dimensional fiber is a consequence of the time-reversal symmetry of the Hamiltonian (1.7) also for $M>1$. Then we determine $\chi(k,t)=(\chi_1(k,t),\dots,\chi_M(k,t))$ as the solution of the equation

$$\partial_t\chi_\alpha(k,t)=[\partial_t P(k,t),P(k,t)]\,\chi_\alpha(k,t)\,.$$

According to Kato [6] $\chi(k,t) = (\chi_1(k,t), \dots, \chi_M(k,t))$ is an orthonormal basis of $\operatorname{Ran} P(k,t)$ and satisfies

$$\langle \chi_\beta(k,t), \partial_t \chi_\alpha(k,t) \rangle = \langle \chi_\beta(k,t), [\partial_t P(k,t), P(k,t)] \chi_\alpha(k,t) \rangle = 0,$$

since

$$\partial_t P(k,t) = P(k,t) \partial_t P(k,t) P(k,t)^\perp + P(k,t)^\perp \partial_t P(k,t) P(k,t).$$

Also, since $P(k,t)$ and $\partial_t P(k,t)$ are equivariant, so are the $\chi_\alpha(k,t)$'s. □

Note that, due to possible band crossings within $\operatorname{Ran} P(k,0)$, the initially chosen smooth basis elements $(\chi_\alpha(k,0))_{\alpha=1}^M$ in general are *not* Bloch functions, *i.e.* they are not eigenfunctions of the operator $H(k,t)$.

Remark 3.7. In the case where $M = 1$, the choice

$$\chi(k,t) = \mathrm{e}^{-\mathrm{i} \int_0^T \phi(s) \mathrm{d}s} \chi(k,0),$$

has the desired property stated in the lemma above.

4. The Super-adiabatic theorem

To perform an approximation of (1.2) to sufficient high order in ε, we need the following so called *super-adiabatic* theorem.
Recall the notation $\mathcal{D}_1 = H^1(\mathbb{T}_y^d)$ and $\mathcal{D}_2 = H^2(\mathbb{T}_y^d)$.

Proposition 4.1. *For each isolated family of Bloch bands $\{E_m(k,t)\}_{m \in M}$, with $M \subset \mathbb{N}$ some finite index set, there exists an equivariant family of projections $P_N^\varepsilon(k,t) \in C^1(I, \mathcal{E}_{L^2(\mathbb{T}^d), \mathcal{D}_2})$ and an equivariant family of unitary operators*

$$T_N^\varepsilon(k,t) : P_N^\varepsilon(k,t)\, L^2(\mathbb{T}^d) \to \mathbb{C}^{|M|}$$

such that $P_N^\varepsilon(k,0) = P(k,0)$, $P_N^\varepsilon(k,T) = P(k,T)$ and the following statements hold:

- **(A) Adiabatic decoupling:** *The propagator $U^\varepsilon(k,t)$ (recall that $t_0 = 0$) of the Schrödinger equation restricted to $\operatorname{Ran} P_N^\varepsilon(k,0) = \operatorname{Ran} P(k,0)$ is close to the adiabatic propagator $U_{\mathrm{a}}^\varepsilon(k,t)$ generated by the adiabatic Hamiltonian*

$$H_{\mathrm{a}}^\varepsilon(k,t) = P_N^\varepsilon(k,t) H(k,t) P_N^\varepsilon(k,t) + \mathrm{i}\varepsilon [\partial_t P_N^\varepsilon(k,t), P_N^\varepsilon(k,t)]$$

up to errors of order ε^N. More precisely we have

$$\| \, (U^\varepsilon(k,t) - U_{\mathrm{a}}^\varepsilon(k,t)) \; P_N^\varepsilon(k,0) \|_{\mathcal{B}(L^2(\mathbb{T}^d), \mathcal{D}_1)} = \mathcal{O}(\varepsilon^N) \tag{4.1}$$

and

$$\| \, (U^\varepsilon(k,t) - U_{\mathrm{a}}^\varepsilon(k,t)) \; P_N^\varepsilon(k,0) \|_{\mathcal{B}(L^2(\mathbb{T}^d), L^2(\mathbb{T}^d))} = \mathcal{O}(\varepsilon^N |t|) \, . \tag{4.2}$$

Since, by construction, $U_{\mathrm{a}}^\varepsilon(k,t) P_N^\varepsilon(k,0) = P_N^\varepsilon(k,t) U_{\mathrm{a}}^\varepsilon(k,t)$, it follows that $\operatorname{Ran} P_N^\varepsilon(k,t)$ is almost invariant under the true time-evolution, i.e.

$$\| \, (\mathbf{1} - P_N^\varepsilon(k,t)) \, U^\varepsilon(k,t) \, P_N^\varepsilon(k,0) \, \|_{\mathcal{B}(L^2(\mathbb{T}^d), \mathcal{D}_1)} = \mathcal{O}(\varepsilon^N) \tag{4.3}$$

and that $P^\varepsilon_N(k,t)$ *approximates* $\rho^\varepsilon(k,t) = U^\varepsilon(k,t)\,P(k,0)\,U^\varepsilon(k,t)^*$,

$$\| P^\varepsilon_N(k,t) - \rho^\varepsilon(k,t) \|_{\mathcal{B}(L^2(\mathbb{T}^d),\mathcal{D}_1)} = \mathcal{O}(\varepsilon^N)\,. \tag{4.4}$$

(B) Effective dynamics: *Let the effective propagator* $U^\varepsilon_{\mathrm{eff}}(k,t)$ *on* $\mathbb{C}^{|M|}$ *be defined by*

$$U^\varepsilon_{\mathrm{eff}}(k,t) := T^\varepsilon_N(k,t)\,U^\varepsilon_{\mathrm{a}}(k,t)\,T^\varepsilon_N(k,0)^*\,,$$

then $U^\varepsilon_{\mathrm{eff}}(k,t)$ *solves the effective Schrödinger equation*

$$\mathrm{i}\,\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\,U^\varepsilon_{\mathrm{eff}}(k,t) = H_{\mathrm{eff}}(k,t)\,U^\varepsilon_{\mathrm{eff}}(k,t)$$

with periodic effective Hamiltonian

$$H_{\mathrm{eff}}(k,t) = \mathbf{E}(k,t) + \mathcal{O}(\varepsilon^2)\,.$$

The self-adjoint $|M|\times|M|$*-matrix* $\mathbf{E}(k,t)$ *is* Γ^**-periodic in* k *and given by*

$$\mathbf{E}_{\alpha\beta}(k,t) = \langle \chi_\alpha(k,t),\ H(k,t)\,\chi_\beta(k,t)\rangle_{L^2(\mathbb{T}^d_y)}\,.$$

Here $(\chi_\alpha(k,t))_{\alpha=1}^M$ *is a basis as in Lemma 3.6, which is used to construct* $T^\varepsilon_N(k,t)$.

If not stated explicitly otherwise, all estimates are uniform for t *in a finite interval.*

Proof. By Assumption 2.1, we have $V_\Gamma \in C^{N+1}(I,\mathcal{B}(H^2(\mathbb{R}^d),L^2(\mathbb{R}^d)))$, which implies, that $(H(\cdot)-\mathrm{i})^{-1} \in C^{N+1}(I,\mathcal{B}(L^2(\mathbb{R}^d),H^2(\mathbb{R}^d)))$, or that $(H(k,\cdot)-\mathrm{i})^{-1} \in C^{N+1}(I,\mathcal{B}(L^2(\mathbb{T}^d),\mathcal{D}_2))$ fiberwise in Bloch-Floquet representation. Hence, according to Proposition 3.5 we have that

$$(H(\cdot,\cdot)-\mathrm{i})^{-1} \in C^{N+1}(I,\mathcal{E}_{L^2(\mathbb{T}^d),\mathcal{D}_2}) \text{ and } P(\cdot,\cdot) \in C^{N+1}(I,\mathcal{E}_{L^2(\mathbb{T}^d),\mathcal{D}_2})\,. \tag{4.5}$$

The projector $P^\varepsilon_N(k,t)$ for *fixed* k is constructed using Nenciu's scheme [13]. For convenience of the reader and in order to observe equivariance we briefly state the result:

Denote the resolvent of $H(k,t)$ at the point $z\in\mathbb{C}$ by $R_z(k,t) = (H(k,t)-z)^{-1}$ and define $P_j(k,t)$, for $j\le N$, recursively via

$$\begin{aligned} P_j(k,t) \;&:=\; G_j(k,t) - 2P_0(k,t)G_j(k,t)P_0(k,t) \\ &\quad + \frac{1}{2\pi}\oint_{C(t)} \mathrm{d}z\, R_z(k,t)\,[P_0(k,t),\partial_t P_{j-1}(k,t)]\;R_z(k,t)\,, \end{aligned}$$

where $C(t)\subset \varrho\,(H(k,t))\subset\mathbb{C}$ is a cycle encircling $\{E_m(k,t)\}_{m\in M}$ once in the positive sense, but no other part of the spectrum of $H(k,t)$, $P_0(k,t) := P(k,t)$ and

$$G_j(k,t) := \sum_{m=1}^{j-1} P_m(k,t)P_{j-m}(k,t)\,.$$

Then

$$\widetilde{P}^\varepsilon_N(k,t) := \sum_{j=0}^{N} \varepsilon^j P_j(k,t)$$

satisfies

$$(\widetilde{P}^\varepsilon_N(k,t)\,)^2 - \widetilde{P}^\varepsilon_N(k,t) = \varepsilon^{N+1} G_{N+1}(k,t) \tag{4.6}$$

as well as

$$\big[\mathrm{i}\varepsilon\partial_t - H(k,t),\, \widetilde{P}^\varepsilon_N(k,t)\big] = \varepsilon^{N+1}\partial_t P_N(k,t)\,. \tag{4.7}$$

From (4.5) and the fact that compositions of equivariant operators are equivariant it follows that $P_j(\cdot,\cdot) \in C^{N+1-j}(I, \mathcal{E}_{L^2(\mathbb{T}^d),\mathcal{D}_2})$ for $j = 1\dots,N$, and thus $\widetilde{P}^\varepsilon_N(\cdot,\cdot) \in C^1(I,\mathcal{E}_{L^2(\mathbb{T}^d),\mathcal{D}_2})$ and also $G_{N+1}(\cdot,\cdot) \in C^1(I,\mathcal{E}_{L^2(\mathbb{T}^d),\mathcal{D}_2})$.
According to (4.6) the spectrum of $\widetilde{P}^\varepsilon_N(k,t)$ is located in ε^{N+1} neighborhoods of 0 and 1. Thus for ε sufficiently small one can define $P^\varepsilon_N(k,t)$ as the spectral projection of $\widetilde{P}^\varepsilon_N(k,t)$ associated with its spectrum near 1, *i.e.*

$$P^\varepsilon_N(k,t) = \frac{\mathrm{i}}{2\pi}\oint_{|z-1|=\frac12} \mathrm{d}z\,(\widetilde{P}^\varepsilon_N(k,t) - z)^{-1}\,.$$

By this definition $P^\varepsilon_N(k,t)$ is obviously a linear operator from $L^2(\mathbb{T}^d)$ into $\mathcal{D}_2$ and an element of $\mathcal{E}_{L^2(\mathbb{T}^d),L^2(\mathbb{T}^d)} \cap \mathcal{E}_{\mathcal{D}_2,\mathcal{D}_2}$. Since $\|P^\varepsilon_N(k,t) - \widetilde{P}^\varepsilon_N(k,t)\| = \mathcal{O}(\varepsilon^{N+1})$, it follows that $\|P^\varepsilon_N(k,t) - P_0(k,t)\| = \mathcal{O}(\varepsilon)$ and hence $\dim(\mathrm{Ran}\, P^\varepsilon_N(k,t))$ $= \dim(\mathrm{Ran}\, P_0(k,t)) = |M| < \infty$. Thus $P^\varepsilon_N(k,t)$ and its derivatives have finite rank, which implies $P^\varepsilon_N(k,t) \in C^1(I,\mathcal{E}_{L^2(\mathbb{T}^d),\mathcal{D}_2})$.
From (4.7) we obtain

$$\begin{aligned}&\big[\mathrm{i}\varepsilon\partial_t - H(k,t),\, P^\varepsilon_N(k,t)\big] = \\ &\quad = -\frac{\mathrm{i}\varepsilon^{N+1}}{2\pi}\oint_{|z-1|=\frac12} \mathrm{d}z\,(\widetilde{P}^\varepsilon_N(k,t)-z)^{-1}\,\partial_t P_N(k,t)\,(\widetilde{P}^\varepsilon_N(k,t)-z)^{-1}.\end{aligned}$$

Hence

$$\big\|\,\big[\mathrm{i}\varepsilon\partial_t - H(k,t),\, P^\varepsilon_N(k,t)\big]\,\big\|_{\mathcal{E}_{L^2(\mathbb{T}^d),\mathcal{D}_2}} = \mathcal{O}(\varepsilon^{N+1}) \tag{4.8}$$

and also

$$\big\|\,\big[\mathrm{i}\varepsilon\partial_t - H(k,t),\, P^\varepsilon_N(k,t)\big]\,\big\|_{\mathcal{E}_{\mathcal{D}_1}} = \mathcal{O}(\varepsilon^{N+1}). \tag{4.9}$$

Now (4.3) follows from Kato's construction [6]. Indeed, let

$$H^\varepsilon_{\mathrm{a}}(k,t) = P^\varepsilon_N(k,t)H(k,t)P^\varepsilon_N(k,t) + \mathrm{i}\varepsilon[P^\varepsilon_N(k,t), \partial_t P^\varepsilon_N(k,t)]$$

be the adiabatic Hamiltonian and $U^\varepsilon_{\mathrm{a}}(k,t)$ the adiabatic evolution generated by $H^\varepsilon_{\mathrm{a}}(k,t)$. Then by construction one has

$$U^\varepsilon_{\mathrm{a}}(k,t)P^\varepsilon_N(k,0) = P^\varepsilon_N(k,t)U^\varepsilon_{\mathrm{a}}(k,t)\,. \tag{4.10}$$

Clearly (4.10) holds for $t=0$ and multiplying both sides by $U^\varepsilon_{\mathrm{a}}(k,t)^*$ and differentiating with respect to t shows that the equality holds for all times.

As a consequence we find that

$$
\begin{aligned}
&(U^\varepsilon(k,t) - U^\varepsilon_{\rm a}(k,t))P^\varepsilon_N(k,0) = \\
&= -U^\varepsilon(k,t)\int_0^t \mathrm{d}s\, \frac{\mathrm{d}}{\mathrm{d}s}\left(U^\varepsilon(k,-s)U^\varepsilon_{\rm a}(k,s)\right) P^\varepsilon_N(k,0) \\
&= -\frac{\mathrm{i}}{\varepsilon}\, U^\varepsilon(k,t)\int_0^t \mathrm{d}s\, U^\varepsilon(k,-s)\left(H^\varepsilon(k,s) - H^\varepsilon_{\rm a}(k,s)\right) P^\varepsilon_N(k,s)U^\varepsilon_{\rm a}(k,s) \\
&= \frac{\mathrm{i}}{\varepsilon}\, U^\varepsilon(k,t)\int_0^t \mathrm{d}s\, U^\varepsilon(k,-s)\big[\mathrm{i}\varepsilon\partial_s - H^\varepsilon(k,s), P^\varepsilon_N(k,s)\big] P^\varepsilon_N(k,s)U^\varepsilon_{\rm a}(k,s) \\
&= \frac{\mathrm{i}}{\varepsilon}\, U^\varepsilon(k,t)\int_0^t \mathrm{d}s\, U^\varepsilon(k,-s)\big[\mathrm{i}\varepsilon\partial_s - H^\varepsilon(k,s), P^\varepsilon_N(k,s)\big] U^\varepsilon_{\rm a}(k,s)P^\varepsilon_N(k,0)\,.
\end{aligned}
$$

As to be shown in Lemma 4.2 below, $U^\varepsilon_{\rm a}(k,t)$ and $U^\varepsilon(k,t)$ are bounded operators from $\mathcal{D}_1$ to $\mathcal{D}_1$. Hence the previous computation together with (4.9) yields (4.1). The statement (4.2) then follows analogously, but since we do not need to invoke Lemma 4.2 below, we additionally obtain an error estimate linear in t. Thus for the full time-evolution we find (4.3),

$$
\begin{aligned}
&\big\|\,(\mathbf{1} - P^\varepsilon_N(k,t))\,U^\varepsilon(k,t)\,P^\varepsilon_N(k,0)\big\|_{\mathcal{B}(L^2(\mathbb{T}^d),\mathcal{D}_1)} = \\
&= \big\|\,(\mathbf{1} - P^\varepsilon_N(k,t))\;(U^\varepsilon(k,t) - U^\varepsilon_{\rm a}(k,t))\;P^\varepsilon_N(k,0)\big\|_{\mathcal{B}(L^2(\mathbb{T}^d),\mathcal{D}_1)} \\
&\le\; \big\|\;(U^\varepsilon(k,t) - U^\varepsilon_{\rm a}(k,t))\;P^\varepsilon_N(k,0)\big\|_{\mathcal{B}(L^2(\mathbb{T}^d),\mathcal{D}_1)} = \mathcal{O}(\varepsilon^N)\,.
\end{aligned}
$$

Lemma 4.2. *$U^\varepsilon(k,t)$, $U^\varepsilon_{\rm a}(k,t) \in \mathcal{B}(\mathcal{D}_1)$ uniformly for $(k,t) \in Y^* \times I$.*

Proof. From Assumption 2.1 and the fact the ∇ is infinitesimally bounded with respect to Δ it follows that there are constants $\mu_\pm, \nu_\pm > 0$ such that for all $\psi \in \mathcal{D}_2$ and $t \in I$

$$
\mu_-\|\nabla\psi\|^2 - \nu_-\|\psi\|^2 \le \langle\psi, H(k,t)\psi\rangle \le \mu_+\|\nabla\psi\|^2 + \nu_+\|\psi\|^2\,.
$$

Hence

$$
\|\psi\|_t^2 := \langle\psi, H(k,t)\psi\rangle_{L^2} + (\nu_- + \mu_-)\|\psi\|^2_{L^2}\,,
$$

defines a norm on $\mathcal{D}_1 = H^1(\mathbb{T}^d)$ which is equivalent to $\|\psi\|^2_{\mathcal{D}_1} := \|\nabla\psi\|^2 + \|\psi\|^2$ uniformly for $t \in I$, since

$$
\mu_-\|\psi\|^2_{\mathcal{D}_1} \le \|\psi\|^2_t \le (\mu_+ + \mu_- + \nu_+ + \nu_-)\|\psi\|^2_{\mathcal{D}_1}\,.
$$

For $\psi_0 \in \mathcal{D}_2$ let $\psi(t) = U^\varepsilon(k,t)\psi_0$. Then by the assumption that $\dot V_\Gamma(y,t)$ is relatively form bounded with respect to Δ there is a constant $c > 0$ such that

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\|\psi(t)\|^2_t &= \langle\psi(t), \dot H(k,t)\psi(t)\rangle \\
&= \langle\psi(t), \dot V_\Gamma(t)\psi(t)\rangle \le c\mu_-\|\psi(t)\|^2_{\mathcal{D}_1} \le c\,\|\psi(t)\|^2_t\,.
\end{aligned}
$$

A Gronwall lemma then yields $\|\psi(t)\|^2_t \le \mathrm{e}^{ct}\|\psi(0)\|^2_0$ and thus we get that $\|U^\varepsilon(k,t)\|_{\mathcal{B}(\mathcal{D}_1)} < \infty$. Since the generators $H(k,t)$ and $H^\varepsilon_{\rm a}(k,t)$ differ only by a bounded operator, the same argument shows that also $U^\varepsilon_{\rm a}(k,t) \in \mathcal{B}(\mathcal{D}_1)$. □

For the construction of the unitary $T^\varepsilon_N(k,t)$ we first choose an orthonormal basis $\big(\chi_1(k,t),\ldots,\chi_{|M|}(k,t)\big)$ of $\operatorname{Ran} P(k,t)$ such that $\chi_\alpha(\cdot,\cdot)\in C^{N+1}(I,\mathcal{E}_{\mathcal{D}_2})$ and

$$\phi_{\alpha\beta}(k,t) = \mathrm{i}\langle \chi_\alpha(k,t), \partial_t \chi_\beta(k,t)\rangle \equiv 0$$

for all $t\in I$, $\alpha,\beta\in\{0,\ldots,|M|\}$. This is always possible as shown in Lemma 3.6. Next we define $T_0(k,t): L^2(\mathbb{T}^d)\to\mathbb{C}^{|M|}$ through

$$(T_0(k,t)\psi)_\alpha = \langle \chi_\alpha(k,t),\, \psi\rangle_{L^2(\mathbb{T}^d_y)}\,.$$

Hence $T_0(\cdot,\cdot)\in C^{N+1}(I,\mathcal{E}_{L^2(\mathbb{T}^d),\mathbb{C}^{|M|}})$. We now give a simplified version of the construction developed in [16]. The idea is again to construct first an asymptotic expansion to the appropriate order. Let

$$\widetilde{T}^\varepsilon_n(k,t) = \sum_{j=0}^n \varepsilon^j T_j(k,t).$$

We require that at order $n\in\mathbb{N}$ it holds that

$$\begin{aligned} \widetilde{T}^\varepsilon_n(k,t)\,\widetilde{T}^\varepsilon_n(k,t)^* - \mathbf{1}_{\mathbb{C}^{|M|}} &= \mathcal{O}(\varepsilon^{n+1})\,,\\ \widetilde{T}^\varepsilon_n(k,t)\,(\mathbf{1}-P^\varepsilon_N(k,t)) &= \mathcal{O}(\varepsilon^{n+1})\,, \end{aligned} \tag{4.11}$$

i.e. that $T^\varepsilon_n(k,t)^*$ is almost unitary as a map from $\mathbb{C}^{|M|}$ to its range and that the range is almost that of $P^\varepsilon_N(k,t)$. Making the ansatz

$$T_j(k,t) = T_0(k,t)\,(a_j(k,t)+b_j(k,t))\,,$$

with self-adjoint $a_j(k,t)$ and anti-self-adjoint $b_j(k,t)$, we find the following recurrence for the coefficients. Clearly (4.11) holds for $n=0$. (For better readability, we drop the (k,t)-dependence in the following, but it is understood that all operators appearing depend on k and t and are equivariant.) Assume that (4.11) holds for n, then

$$\widetilde{T}^\varepsilon_n\,\widetilde{T}^{\varepsilon *}_n - \mathbf{1}_{\mathbb{C}^{|M|}} = \varepsilon^{n+1}\sum_{k=1}^n T_k T^*_{n+1-k} + \mathcal{O}(\varepsilon^{n+2}) =: \varepsilon^{n+1}\,A_{n+1} + \mathcal{O}(\varepsilon^{n+2})$$

and thus T_{n+1} has to solve

$$T_0 T^*_{n+1} + T_{n+1}T^*_0 = 2T_0\,a_{n+1}\,T^*_0 \stackrel{!}{=} -A_{n+1}\,. \tag{4.12}$$

Hence, one must choose

$$a_{n+1} = -\tfrac12 T^*_0 A_{n+1} T_0\,.$$

Again by the induction assumption

$$\begin{aligned} &(\widetilde{T}^\varepsilon_n + \varepsilon^{n+1}T_0 a_{n+1})(\mathbf{1}-P^\varepsilon_N) = \\ &= \; -\varepsilon^{n+1}\sum_{j=0}^n \big(T_j P_{n+1-j} - \tfrac12 A_{n+1}T_0(\mathbf{1}-P_0)\big) + \mathcal{O}(\varepsilon^{n+2})\\ &= \; -\varepsilon^{n+1}\sum_{j=0}^n T_j P_{n+1-j} + \mathcal{O}(\varepsilon^{n+2})\\ &=: \; \varepsilon^{n+1}B_{n+1} + \mathcal{O}(\varepsilon^{n+2})\,. \end{aligned}$$

Thus b_{n+1} has to solve

$$T_0 b_{n+1}(\mathbf{1}-P_0) = -B_{n+1} = -B_{n+1}(\mathbf{1}-P_0) + \mathcal{O}(\varepsilon)\,,$$

where the last equality follows by multiplying the previous equation with P_N^ε from the right. A possible choice is therefore

$$b_{n+1} = -T_0^* B_{n+1}(\mathbf{1}-P_0)\,,$$

which leaves us with the following recurrence relation

$$T_{n+1} = -\frac{1}{2}\sum_{k=1}^{n} T_k T^*_{n+1-k} T_0 + \sum_{j=0}^{n} T_j P_{n+1-j}(\mathbf{1}-P_0),$$

up to $n+1=N$. Then by construction $\widetilde{T}_N^\varepsilon(\cdot,\cdot) \in C^1(I, \mathcal{E}_{L^2(\mathbb{T}^d),\mathbb{C}^{|M|}})$ and

$$\begin{aligned} \widetilde{T}_N^\varepsilon(k,t)\,\widetilde{T}_N^\varepsilon(k,t)^* - \mathbf{1}_{\mathbb{C}^{|M|}} &= \mathcal{O}(\varepsilon^{N+1}), \\ \widetilde{T}_N^\varepsilon(k,t)\,(\mathbf{1} - P_N^\varepsilon(k,t)) &= \mathcal{O}(\varepsilon^{N+1})\,. \end{aligned}$$

In order to construct a true unitary observe that $\widetilde{T}_N^\varepsilon\,\widetilde{T}_N^{\varepsilon\,*}$ is a positive self-adjoint operator $\mathcal{O}(\varepsilon^{N+1})$-close to the identity. Hence

$$\hat{T}_N^\varepsilon = \left(\widetilde{T}_N^\varepsilon\,\widetilde{T}_N^{\varepsilon\,*}\right)^{-\frac{1}{2}}\widetilde{T}_N^\varepsilon$$

is a unitary operator $\mathcal{O}(\varepsilon^{N+1})$-close to $\widetilde{T}_N^\varepsilon$. Finally let

$$T_N^\varepsilon = \left(\hat{T}_N^\varepsilon\,P_N^\varepsilon\,\hat{T}_N^{\varepsilon\,*}\right)^{-\frac{1}{2}}\,\hat{T}_N^\varepsilon\,P_N^\varepsilon\,,$$

which implies $T_N^\varepsilon\,T_N^{\varepsilon\,*} = P_N^\varepsilon$ and again $T_N^\varepsilon(\cdot,\cdot) \in C^1(I, \mathcal{E}_{L^2(\mathbb{T}^d),\mathbb{C}^{|M|}})$

We conclude that $P_N^\varepsilon(k,t)$ and $T_N^\varepsilon(k,t)$ are equivariant by construction and have an explicit expansion up to terms of order $\mathcal{O}(\varepsilon^{N+1})$ given by

$$P_N^\varepsilon(k,t) = \sum_{j=0}^{N}\varepsilon^j P_j(k,t) + R^\varepsilon_{P,N+1}(k,t)$$

and

$$T_N^\varepsilon(k,t) = \sum_{j=0}^{N}\varepsilon^j T_j(k,t) + R^\varepsilon_{T,N+1}(k,t)\,,$$

where

$$\|R^\varepsilon_{P,N+1}(k,t)\|_{\mathcal{E}} = \mathcal{O}(\varepsilon^{N+1}) \quad \text{and} \quad \|R^\varepsilon_{T,N+1}(k,t)\|_{\mathcal{E}} = \mathcal{O}(\varepsilon^{N+1})\,.$$

In particular we have

$$P_1(k,t) = \frac{1}{2\pi}\oint_{C(t)} \mathrm{d}z\,R_z(k,t)\,[P_0(k,t), \partial_t P_0(k,t)]\;R_z(k,t)$$

and

$$T_1(k,t) = T_0(k,t)\,P_1(k,t)\,(\mathbf{1} - P_0(k,t))\,,$$

which yields $T_1 P_0 = T_0 P_1 P_0 = 0$. Now

$$\begin{aligned} H^\varepsilon_{\mathrm{eff}}(k,t) := {} & T_N^\varepsilon(k,t)\,P_N^\varepsilon(k,t)\,H(k,t)\,P_N^\varepsilon(k,t)\,T_N^\varepsilon(k,t)^* \\ & - \mathrm{i}\varepsilon\,T_N^\varepsilon(k,t)\,\partial_t T_N^\varepsilon(k,t)^* \end{aligned}$$

defines a self-adjoint and periodic operator on $\mathbb{C}^{|M|}$, which depends continuously on t. More precisely, $H^\varepsilon_{\rm eff}(\cdot,\cdot) \in C(I, \mathcal{E}_{\mathbb{C}^{|M|},\mathbb{C}^{|M|}})$. Due to the particular choice of our basis $(\chi_\alpha(k,t))_{\alpha=1}^M$, constructed in Lemma 3.6, we get that

$$\begin{aligned} T_N^\varepsilon(k,t)\,\partial_t T_N^\varepsilon(k,t)^* &= \sum_\alpha |e_\alpha\rangle\langle\chi_\alpha(k,t)| \sum_\beta |\partial_t\chi_\beta(k,t)\rangle\langle e_\beta| + \mathcal{O}_{\mathcal{E}}(\varepsilon) \\ &= \mathcal{O}_{\mathcal{E}}(\varepsilon). \end{aligned}$$

Therefore, $T_1 P_0 = T_0 P_1 P_0 = 0$ implies

$$\begin{aligned} H^\varepsilon_{\rm eff}(k,t) &= T_0(k,t)P_0(k,t)H(k,t)P_0(k,t)T_0(k,t)^* + \mathcal{O}_{\mathcal{E}}(\varepsilon^2) \\ &= \mathbf{E}(k,t) + \mathcal{O}_{\mathcal{E}}(\varepsilon^2)\,. \end{aligned}$$

Since

$$T_N^\varepsilon(k,t)\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} - H^\varepsilon_{\rm a}(k,t)\right)T_N^\varepsilon(k,t)^* = \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t} - H^\varepsilon_{\rm eff}(k,t)\,,$$

it follows that

$$U^\varepsilon_{\rm a}(k,t)\,T_N^{\varepsilon\,*}(k,0) = T_N^{\varepsilon\,*}(k,t)U^\varepsilon_{\rm eff}(k,t)\,, \tag{4.13}$$

which concludes the proof. □

5. Proof of the main results

While Theorem 2.3 follows directly from the super-adiabatic approximation (4.4) of the state at time t, the semiclassical approximation of Theorem 2.4 is based on the effective dynamics in the almost invariant subspace.

5.1. **Proof of Theorem 2.3.**

We first note that the state

$$\rho^\varepsilon(k,t) = U^\varepsilon(k,t)P(k,0)U^\varepsilon(k,t)^*$$

at time $t \in I$ as well as the current operator J^ε defined in (1.3) are fibered,

$$\mathcal{Z}J^\varepsilon\mathcal{Z}^{-1}(k) = \frac{1}{\varepsilon}\,(-\mathrm{i}\nabla_y + k) = \frac{\mathrm{i}}{\varepsilon}\,[H(k,t), \mathrm{i}\nabla_k^\tau]\,.$$

Since $\rho^\varepsilon(k,t)$ has finite dimensional range contained in $\mathcal{D}_1$, $\rho^\varepsilon(k,t)\,J^\varepsilon(k)$ is trace class and, invoking Lemma 3.3, the macroscopic current in the state $\rho^\varepsilon(t)$ is given by

$$\dot{\mathbf{P}}^\varepsilon(t) = \frac{1}{(2\pi)^d}\int_{\mathbb{T}^*}\mathrm{d}k\ \mathrm{Re}\,\mathrm{tr}\,\rho^\varepsilon(k,t)J^\varepsilon(k) = \frac{1}{(2\pi)^d}\int_{\mathbb{T}^*}\mathrm{d}k\ \mathrm{tr}\,\rho^\varepsilon(k,t)J^\varepsilon(k)\,.$$

The integrand can be evaluated as follows: First observe that with (4.4)

$$\begin{aligned} \mathrm{tr}\,\rho^\varepsilon(k,t)\,J^\varepsilon(k) &= \mathrm{tr}\,P_N^\varepsilon(k,t)\,J^\varepsilon(k) + \mathcal{O}(\varepsilon^N) \\ &= \frac{\mathrm{i}}{\varepsilon}\,\mathrm{tr}\,P_N^\varepsilon(k,t)[H(k,t), \mathrm{i}\nabla_k^\tau]P_N^\varepsilon(k,t) + \mathcal{O}(\varepsilon^N). \end{aligned}$$

Next we compute using (4.8) that

$$\begin{aligned}P_N^\varepsilon\, H\,\mathrm{i}\nabla_k^\tau\, P_N^\varepsilon &= P_N^\varepsilon\, H\, P_N^\varepsilon\,\mathrm{i}\nabla_k^\tau + \mathrm{i}P_N^\varepsilon\, H\,(\nabla_k P_N^\varepsilon)\,(P_N^\varepsilon + \mathbf{1} - P_N^\varepsilon)\\ &= P_N^\varepsilon\, H\, P_N^\varepsilon\,\mathrm{i}\nabla_k^\tau\ - \mathrm{i}P_N^\varepsilon\,[H, P_N^\varepsilon]\,(\nabla_k P_N^\varepsilon)\,P_N^\varepsilon\\ &\quad + \mathrm{i}P_N^\varepsilon\, H\,(\nabla_k P_N^\varepsilon)\,(\mathbf{1} - P_N^\varepsilon)\\ &= P_N^\varepsilon\, H\, P_N^\varepsilon\,\mathrm{i}\nabla_k^\tau + \varepsilon\, P_N^\varepsilon\,\dot P_N^\varepsilon\,(\nabla_k P_N^\varepsilon)\,P_N^\varepsilon\\ &\quad + \mathrm{i}P_N^\varepsilon\, H\,(\nabla_k P_N^\varepsilon)\,(\mathbf{1} - P_N^\varepsilon) + \mathcal{O}_{\mathcal{E}}(\varepsilon^{N+1})\end{aligned}$$

and therefore

$$\begin{aligned}P_N^\varepsilon\,[H,\,\mathrm{i}\nabla_k^\tau]\,P_N^\varepsilon &= P_N^\varepsilon\, H\,\mathrm{i}\nabla_k^\tau\, P_N^\varepsilon - (P_N^\varepsilon\, H\,\mathrm{i}\nabla_k^\tau\, P_N^\varepsilon)^*\\ &= [P_N^\varepsilon\, H\, P_N^{\varepsilon *},\,\mathrm{i}\nabla_k^\tau\,] + \varepsilon\, P_N^\varepsilon\,[\dot P_N^\varepsilon,\,(\nabla_k P_N^\varepsilon)]\,P_N^\varepsilon\\ &\quad + R_N^\varepsilon + \mathcal{O}_{\mathcal{E}}(\varepsilon^{N+1})\\ &= -\,\mathrm{i}(\nabla_k P_N^\varepsilon\, H\, P_N^\varepsilon) + \varepsilon\, P_N^\varepsilon\,[\dot P_N^\varepsilon,\,(\nabla_k P_N^\varepsilon)]\,P_N^\varepsilon\\ &\quad + R_N^\varepsilon + \mathcal{O}_{\mathcal{E}}(\varepsilon^{N+1})\,,\end{aligned}$$

where $\mathrm{Tr}\, R_N^\varepsilon(k,t) = 0$ for all $t \in I$ and $k \in \mathbb{T}^*$. We take the trace for fixed k and abbreviate $\mathbf{E}^\varepsilon(k,t) = P_N^\varepsilon(k,t)\, H(k,t)\, P_N^\varepsilon(k,t)$ to obtain

$$\begin{aligned}\mathrm{tr}\,(P_N^\varepsilon(k,t)[H(k,t),\mathrm{i}\nabla_k^\tau]P_N^\varepsilon(k,t)) = &-\mathrm{i}\nabla_k\,\mathrm{tr}\,\mathbf{E}^\varepsilon(k,t)\\ &+ \varepsilon\,\mathrm{tr}\,(P_N^\varepsilon(k,t)[\partial_t P_N^\varepsilon(k,t), \nabla_k P_N^\varepsilon(k,t)])\\ &+ \mathcal{O}(\varepsilon^{N+1}).\end{aligned}$$

In summary we just computed that

$$\mathrm{tr}\,\rho^\varepsilon(k,t)J^\varepsilon(k) = \frac{1}{\varepsilon}\nabla_k\,\mathrm{tr}\,\mathbf{E}^\varepsilon(k,t) + \mathrm{i}\,\mathrm{tr}\,P_N^\varepsilon(k,t)[\partial_t P_N^\varepsilon(k,t), \nabla_k P_N^\varepsilon(k,t)] + \mathcal{O}(\varepsilon^N).$$

By exploiting the fact that $\mathrm{tr}\,\mathbf{E}^\varepsilon(k,t)$ is a periodic function of k,

$$\mathrm{tr}\,\mathbf{E}^\varepsilon(k-\gamma^*,t) = \mathrm{tr}\,\tau(\gamma^*)\,\mathbf{E}^\varepsilon(k,t)\,\tau(\gamma^*)^{-1} = \mathrm{tr}\,\mathbf{E}^\varepsilon(k,t) \quad \forall\,\gamma^* \in \Gamma^*\,,$$

we finally get

$$\begin{aligned}\dot{\mathbf{P}}^\varepsilon(t) &= \frac{1}{(2\pi)^d}\int_{\mathbb{T}^*}\mathrm{d}k\ \mathrm{tr}\,(\rho^\varepsilon(k,t)J^\varepsilon(k))\\ &= \frac{\mathrm{i}}{(2\pi)^d}\int_{\mathbb{T}^*}\mathrm{d}k\ \mathrm{tr}\,(P_N^\varepsilon(k,t)[\partial_t P_N^\varepsilon(k,t), \nabla_k P_N^\varepsilon(k,t)]) + \mathcal{O}(\varepsilon^N)\,,\end{aligned}$$

which proves formula (2.1) in Theorem 2.3.

To conclude (2.3), we observe that evaluating the traces in the definitions of the curvatures $\Theta(k,t)$ and $\Theta_N^\varepsilon(k,t)$ with respect to the orthonormal basis $(\chi_\alpha(k,t))_{\alpha=1}^M$ of $\mathrm{Ran}\,P(k,t)$ resp. the orthonormal basis $(\chi_\alpha^\varepsilon(k,t))_{\alpha=1}^M = (T_N^{\varepsilon *}(k,t)\,T_0(k,t)\chi_\alpha(k,t))_{\alpha=1}^M$ of $\mathrm{Ran}\,P_N^\varepsilon(k,t)$ yields

$$\begin{aligned}\Theta(k,t) &= -\,\mathrm{i}\,\mathrm{tr}\,(P(k,t)\,[\partial_t P(k,t),\,\nabla_k P(k,t)])\\ &= 2\mathrm{i}\sum_\alpha \mathrm{Im}\,\langle\partial_t\chi_\alpha(k,t), \nabla_k\chi_\alpha(k,t)\rangle\end{aligned}$$

and likewise for $\Theta^\varepsilon_N(k,t)$,

$$\begin{aligned}\Theta^\varepsilon_N(k,t) = &\; -\mathrm{i}\,\mathrm{tr}\left(P^\varepsilon_N(k,t)\left[\partial_t P^\varepsilon_N(k,t),\ \nabla_k P^\varepsilon_N(k,t)\right]\right)\\ = &\; 2\mathrm{i}\sum_\alpha \mathrm{Im}\,\langle \partial_t \chi^\varepsilon_\alpha(k,t), \nabla_k \chi^\varepsilon_\alpha(k,t)\rangle\ .\end{aligned}$$

Thus we obtain $\Theta(k,t) = -\partial_t \mathcal{A}(k,t) - \nabla_k \phi(k,t)$, where the geometric vector potentials is

$$\mathcal{A}(k,t) = \mathrm{i}\sum_\alpha \langle \chi_\alpha(k,t), \nabla_k \chi_\alpha(k,t)\rangle\ ,$$

and the geometric scalar potential is

$$\phi(k,t) = -\mathrm{i}\sum_\alpha \langle \chi_\alpha(k,t), \partial_t \chi_\alpha(k,t)\rangle\ .$$

The decomposition for $\Theta^\varepsilon_N(k,t)$ in terms of $\mathcal{A}^\varepsilon_N(k,t)$ and $\phi^\varepsilon_N(k,t)$ is then completely analogous with $\chi^\varepsilon_\alpha(k,t)$ replacing $\chi_\alpha(k,t)$. By construction we have that $T^\varepsilon_N(k,0) = T_0(k,0)$ and $T^\varepsilon_N(k,T) = T_0(k,T)$ and therefore $\chi_\alpha(k,0) = \chi^\varepsilon_\alpha(k,0)$, as well as $\chi_\alpha(k,T) = \chi^\varepsilon_\alpha(k,T)$. As a consequence also $\mathcal{A}^\varepsilon_N(k,0) = \mathcal{A}(k,0)$ and $\mathcal{A}^\varepsilon_N(k,T) = \mathcal{A}(k,T)$. Hence

$$\begin{aligned}-\int_0^T \mathrm{d}t \int_{\mathbb{T}^*} \mathrm{d}k\, \Theta^\varepsilon_N(k,t) &= \int_0^T \mathrm{d}t \int_{\mathbb{T}^*} \mathrm{d}k\, \left(\partial_t \mathcal{A}^\varepsilon_N(k,t) + \nabla_k \phi^\varepsilon_N(k,t)\right)\\ &= \int_{\mathbb{T}^*} \mathrm{d}k\ \left(\mathcal{A}^\varepsilon_N(k,T) - \mathcal{A}^\varepsilon_N(k,0)\right)\\ &= \int_{\mathbb{T}^*} \mathrm{d}k\ \left(\mathcal{A}(k,T) - \mathcal{A}(k,0)\right)\\ &= -\int_0^T \mathrm{d}t \int_{\mathbb{T}^*} \mathrm{d}k\, \Theta(k,t)\,,\end{aligned}$$

where the second equality follows from the periodicity of $\phi^\varepsilon_N(k,t)$ in k and for the last equality one just reverses the preceding steps for the adiabatic instead of the superadiabatic quantities. □

5.2. **Proof of Theorem 2.4.** In the proof of our second result we will make heavy use of the semiclassical calculus for operators with equivariant symbols as presented in [16, 23]. The reader is referred to these references for more details as we shall hereafter use the developed semiclassical techniques without any further ado.

In the following we consider the case where all Bloch bands within $\mathrm{Ran}\,P(k,t)$, $t \in I$, are isolated and non-degenerated. It suffices then to restrict ourselves to only one of these bands. Thus, the results of Section 4 yield an effective Hamiltonian $H_{\mathrm{eff}}(k,t)$, acting as a simple multiplication operator on the reference space $L^2(\mathbb{T}^*, \mathbb{C})$, such that

$$H_{\mathrm{eff}}(k,t) = E_m(k,t) + \mathcal{O}_{\mathcal{E}}(\varepsilon^2). \tag{5.1}$$

The corresponding classical equations of motion are simply given by

$$\begin{cases} \dot r = \nabla_k E_m(k,t), \\ \dot k = 0, \end{cases} \tag{5.2}$$

and the generated classical flow will be denoted by

$$\widetilde{\Phi}_m(t,0) : (k,\, r) \mapsto \left(k,\, r + \int_0^t \mathrm{d}s\, \nabla_k E_m(k,s) \right). \tag{5.3}$$

To conclude the proof of Theorem 2.4 we need one more additional result, namely the following Egorov-type theorem for time-dependent Hamiltonians.

Lemma 5.1. *Let $E_m(t)$ be an isolated and non-degenerated Bloch band for all $t \in I$. Denote by*

$$U_m^\varepsilon(k,t) = \exp\left(-\frac{\mathrm{i}}{\varepsilon} \int_0^t \mathrm{d}s\, E_m(k,s) \right)$$

the unitary propagator associated to $E_m(k,t)$. Then, for any $a \in C_\mathrm{b}^\infty$ there is a $C_a < \infty$ such that

$$\left\| U_m^\varepsilon(k,t)^*\, a^W\, U_m^\varepsilon(k,t) - (a \circ \widetilde{\Phi}_m(t,0))^W \right\| \leq \varepsilon^2 C_a |t|(1+|t|), \tag{5.4}$$

where $\widetilde{\Phi}_m(t,0)$ is given by (5.3).

Proof. The proof is almost analogous to the time-independent case, nevertheless it is given here for completeness. First note that the function $E_m(k,s)$ is bounded together with its partial derivatives (on bounded time intervals). Having in mind (5.3), we note that $(a \circ \widetilde{\Phi}_m(t,0)) \in C_\mathrm{b}^\infty$, as well as $\partial_t (a \circ \widetilde{\Phi}_m(t,0)) \in C_\mathrm{b}^\infty$, for any fixed $t \in \mathbb{R}$. We therefore can interchange quantization and differentiation w.r.t. $t \in \mathbb{R}$ and write

$$\begin{aligned} &U_m^\varepsilon(k,t)^*\, a^W\, U_m^\varepsilon(t,k) - (a \circ \widetilde{\Phi}_m(t,0))^W = \\ &= \int_0^t \mathrm{d}s \, \frac{\mathrm{d}}{\mathrm{d}s} \left(U_m^\varepsilon(k,s)^* \, (a \circ \widetilde{\Phi}_m(t,s))^W \, U_m^\varepsilon(s,k) \right) \\ &= \int_0^t \mathrm{d}s \, U_m^\varepsilon(k,s)^* \, I(t,s) \, U_m^\varepsilon(k,s) \, . \end{aligned}$$

where we denote

$$I(t,s) \equiv \frac{\mathrm{i}}{\varepsilon} \left[E_m(k,s), (a \circ \widetilde{\Phi}_m(t,s))^W \right] + \frac{\mathrm{d}}{\mathrm{d}s} (a \circ \widetilde{\Phi}_m(t,s))^W.$$

Having in mind (5.3), we easily get

$$\frac{\mathrm{d}}{\mathrm{d}s} (a \circ \widetilde{\Phi}_m(t,s)) = -\nabla_k E_m(k,s) \cdot \nabla_r (a \circ \widetilde{\Phi}_m(t,s)).$$

Thus we can use Moyal's expansion of the commutator, to obtain

$$\frac{\mathrm{i}}{\varepsilon} \left[E_m(k,s), (a \circ \widetilde{\Phi}_m(t,s)) \right]_\sharp - \nabla_k E_m(k,s) \cdot \nabla_r (a \circ \widetilde{\Phi}_m(t,s)) = \mathcal{O}(\varepsilon^2),$$

where $\sharp$ denotes the Moyal product of symbols. Moreover, by using the the simple time-dependence of the classical flow (5.3), we also obtain that the integrand $I(t,s)$ is indeed $\mathcal{O}(\varepsilon^2(1+|t-s|))$, since derivatives w.r.t k of $(a \circ \widetilde{\Phi}_m(t,s))$ grow linearly in time for large enough t. This fact together with the consequent integration in time of $I(t,s)$ then proves assertion of the lemma. ∎

Proof of Theorem 2.4. The above given lemma is stated in terms of observables on the reference space $L^2(\mathbb{T}^*, \mathbb{C})$. In order to obtain the analogous result in the physical phase space and the correpsonding effective semiclassical equations of motion (2.10) we have to undo both, the mapping to the reference space T_N^ε as well as the Bloch-Floquet transformation $\mathcal{Z}$. To this end, Moyal's expansion will allow us to derive explicit formulas up to sufficient high orders in ε.

Let us first study how the Bloch-Floquet transformation $\mathcal{Z}$ maps observables on $\mathcal{H} = L^2(\mathbb{R}^d)$ to observables in the corresponding Zak representation. From [16], we know that

$$\mathcal{Z}^{-1}\, a^W(\mathrm{i}\varepsilon\nabla_k^\tau, k)\, \mathcal{Z} = a^W(\varepsilon x, -\mathrm{i}\nabla_x) \tag{5.5}$$

whenever $a(r,k) \equiv a(r, k+\gamma^*)\ \forall\ \gamma \in \Gamma^*$. Here $a^W(\varepsilon x, -\mathrm{i}\nabla_x)$ denotes the Weyl quantized operator acting on $L^2(\mathbb{R}^d, \mathbb{C})$, whereas the operator $a^W(\mathrm{i}\varepsilon\nabla_k^\tau, k)$ acts on $L^2(Y^*, L^2(\mathbb{T}^d))$. One should note confuse these two types of quantization, even though they are both obtained from the same symbol $a(r,k)$. Moreover $a^W(\mathrm{i}\varepsilon\nabla_k^\tau, k)$, *i.e.* observables in the Zack representation, should be distinguished from observables $a^W(\mathrm{i}\varepsilon\nabla_k, k)$ acting on the reference space $L^2(\mathbb{T}^*, \mathbb{C})$.

Next we define a change of coordinates (for each fixed $t \in \mathbb{R}$) by

$$\Sigma_t^\varepsilon : \mathbb{R}^{2d} \to \mathbb{R}^{2d}, \quad (r,k) \mapsto (r + \varepsilon\mathcal{A}_m(k,t), k), \tag{5.6}$$

where $\mathcal{A}_m(k,t)$ is the Berry connection, as defined in (1.13). We claim that the unitary operator $T_N^\varepsilon(t) : P_N^\varepsilon(t)\, L^2(Y^*, L^2(\mathbb{T}^d)) \to L^2(Y^*)$ constructed in Proposition 4.1 maps semiclassical observables in the Bloch-Floquet representation to observables in the reference space via

$$T_N^\varepsilon(t)\, a^W\, T_N^{\varepsilon\,*}(t) = ((a \circ \Sigma_t^\varepsilon)(k,r))^W + \mathcal{O}(\varepsilon^2), \tag{5.7}$$

where here and in the following $\mathcal{O}(\varepsilon^n)$ refers to the norm of bounded operators. This formula should be compared to (5.5): Whereas $\mathcal{Z}$ leaves the semiclassical symbol $a(r,k)$ invariant, the unitary mapping to the reference space T_N^ε does not. This can be seen by using Moyal's expansion, *i.e.* we have to expand

$$T_N^\varepsilon(k,t)\, \sharp\, a(r,k)\, \sharp\, T_N^{\varepsilon\,*}(k,t)$$

in powers of ε. To this end recall that we explicitly constructed $T_N^\varepsilon = T_0 + \varepsilon\, T_1 + \mathcal{O}_\mathcal{E}(\varepsilon^2)$ in the proof of Proposition 4.1 above and that the equivariance property of $T_N^\varepsilon(k,t)$ assures that we can interpret $T_N^\varepsilon(k,t)$ as an operator valued semiclassical symbol in the sense of [16, 23] with quantization $T_N^\varepsilon(t)$. Since $a(r,k)$ is scalar-valued, a straightforward calculation yields

$$\begin{aligned} T_N^\varepsilon(k,t)\, \sharp\, a(r,k)\, \sharp\, T_N^{\varepsilon\,*}(k,t) &= a(r,k) + \mathrm{i}\varepsilon\, \nabla_r a(r,k) \cdot T_0(k,t) \nabla_k T_0^*(k,t) \\ &\quad + \mathcal{O}(\varepsilon^2), \end{aligned}$$

where we have used that $T_N^\varepsilon(k,t)$ does *not* depend on r and the fact that

$$T_0(k,t) T_1^*(k,t) + T_1(k,t) T_0^*(k,t) = 0,$$

by relation (4.12). A comparison with the Taylor expansion in powers of ε for $a \circ \Sigma_t^\varepsilon$ proves the claim.

Combining (5.5) and (5.7) allows us to transform the Egorov theorem 5.1 into the corresponding result on the original Hilbert space $L^2(\mathbb{R}^d)$ and thus to conclude the assertion of Theorem 2.4. To this end we write

$$P(0)\, U^\varepsilon(t)^*\, a^W\, U^\varepsilon(t)\, P(0) = \mathcal{Z}^{-1} P_N^\varepsilon(0)\, U^\varepsilon(t)^*\, a^W\, U^\varepsilon(t)\, P_N^\varepsilon(0)\mathcal{Z}.$$

Invoking Proposition 4.1 we obtain

$$\begin{aligned} &P_N^\varepsilon(0)\, U^\varepsilon(t)^*\, a^W\, U^\varepsilon(t)\, P_N^\varepsilon(0) = \\ &= T_N^\varepsilon(0)\, U_{\mathrm{a}}^\varepsilon(t)^*\, a^W\, U_{\mathrm{a}}^\varepsilon(t)\, T_N^{\varepsilon *}(0) + \mathcal{O}(\varepsilon^N) \\ &= U_m^\varepsilon(t)^*\, T_N^\varepsilon(t)^*\, a^W\, T_N^\varepsilon(t)^*\, U_m^\varepsilon(t)\; + \mathcal{O}(\varepsilon^N) \\ &= U_m^\varepsilon(t)^*\, (a\circ\Sigma_t^\varepsilon)^W\, U_m^\varepsilon(t) + \mathcal{O}(\varepsilon^2), \end{aligned}$$

where for the last equality we simply inserted (5.7). By Lemma 5.1, this yields

$$\begin{aligned} &P_N^\varepsilon(0)\, U_m^\varepsilon(t)^*\, (a\circ\Sigma_t^\varepsilon)^W\, U_m^\varepsilon(t)\, P_N^\varepsilon(0) = \\ &= P_N^\varepsilon(0)\left((a\circ\Sigma_t^\varepsilon)\circ\widetilde{\Phi}_m^\varepsilon(t,0)\right)^W P_N^\varepsilon(0) + \mathcal{O}(\varepsilon^2|t|(1+|t|)) \\ &= P_N^\varepsilon(0)\left((b\circ\Phi_m^\varepsilon(t,0))\circ\Sigma_t^\varepsilon\right)^W P_N^\varepsilon(0) + \mathcal{O}(\varepsilon^2|t|(1+|t|)), \end{aligned}$$

where we define the classical flow, which maps observables on physical phase space, via

$$\Phi_m^\varepsilon(t,0) := \Sigma_t\circ\widetilde{\Phi}_m^\varepsilon(t,0)\circ\Sigma_t^{-1}.$$

Thus we denote the new coordinates $(q,p)\in\mathbb{R}^{2d}$ by

$$q = r + \varepsilon\mathcal{A}_m(k,t), \quad p = k.$$

Using (5.2), it is then straightforward to express Hamilton's equations of motion (in the mth Bloch band) in these new coordinates, *i.e.*

$$\dot q = \nabla_p E_m(p,t) - 2\varepsilon\,\mathrm{Im}\,\langle\partial_t\varphi_m(p,t),\nabla_p\varphi_m(p,t)\rangle\,, \qquad \dot p = 0,$$

and since, as before,

$$\mathrm{Im}\,\langle\partial_t\varphi_m(k,t),\nabla_k\varphi_m(k,t)\rangle = -\frac{\mathrm{i}}{2}\,\mathrm{tr}\left(P_m(k,t)\left[\partial_t P_m(k,t),\,\nabla_k P_m(k,t)\right]\right),$$

we clearly get (2.10). In summary this yields

$$\left\| P_m(0)\left(U^\varepsilon(t)^*\, a^W\, U^\varepsilon(t) - (a\circ\Phi_m^\varepsilon(t,0))^W\right) P_m(0)\right\| \le C\varepsilon^2|t|(1+|t|),$$

or, in other words, for any $\psi_0\in\mathrm{Ran}\,P_m(0)$ we get

$$\left|\langle\psi_0, U^\varepsilon(t)^*\, a^W\, U^\varepsilon(t)\,\psi_0\rangle_{L^2} - \langle\psi_0,(a\circ\Phi_m^\varepsilon(t,0))^W\,\psi_0\rangle_{L^2}\right| \le C\varepsilon^2|t|(1+|t|).$$

Finally, by using identity (2.9), we convert this Egorov type theorem for operators into the analogous one for Wigner functions, *cf.* [24], having in mind that Φ_m^ε is volume preserving. Thus Theorem 2.4 is proved. □

6. Symmetries and geometric interpretation of currents

6.1. **Symmetries.** In many physical problems, the role of symmetries is crucial for a deep understanding of the dynamics. Piezoelectricity is no exception. Indeed we prove that the piezoelectric current is zero *if space-reflection symmetry is not broken*, in agreement with the common lore in solid state physics.

As usual, space-reflection symmetry is realized in $\mathcal{H} = L^2(\mathbb{R}^d)$ by the operator $\mathscr{R}$, defined by

$$(\mathscr{R}\psi)(x) = \psi(-x), \qquad \psi \in L^2(\mathbb{R}^d).$$

The group structure of the periodicity lattice Γ implies that $-\Gamma = \Gamma$, *i.e.* that for any $\gamma \in \Gamma$ one has $-\gamma \in \Gamma$. Therefore $[-x] = -[x] \in Y$, where we introduce $x = [x] + \gamma$ for the a.e. unique decomposition for $x \in \mathbb{R}^d$ as a sum of $[x] \in Y$ and $\gamma \in \Gamma$. Equipped with this observation it is easy to check that $\widetilde{\mathscr{R}} = \mathcal{Z}\mathscr{R}\mathcal{Z}^{-1}$ acts as

$$\left(\widetilde{\mathscr{R}}\psi\right)(k,y) = \psi(-k,-y), \qquad \psi \in L^2(Y_k^*) \otimes \mathcal{H}_{\mathrm{f}},$$

or equivalently $(\widetilde{\mathscr{R}}\psi)(k) = \mathscr{R}_{\mathrm{f}}\psi(-k)$ where $\mathscr{R}_{\mathrm{f}}$ is the space reflection operator in $\mathcal{H}_{\mathrm{f}} = L^2(\mathbb{T}_y^d)$.

Notice that, if $H(t) = -\frac{1}{2}\Delta + V_\Gamma(t,x)$, then the condition $[H(t), \mathscr{R}] = 0$ is fulfilled whenever $V_\Gamma(t,-x) = V_\Gamma(t,x)$. Some authors refer to this condition by saying that *the crystal has a center of inversion.* However, the use of the world "crystal" should not obscure the fact that the latter is a property of V_Γ, not a property of Γ.

Proposition 6.1 (**Space-reflection symmetry**)**.** *Assume that the self-adjoint operator $H(t)$ commutes with $\mathscr{R}$, and that $\mathcal{Z}H(t)\mathcal{Z}^{-1}$ is a* continuously *fibered operator. Let $P(\cdot,t)$ be either*

(a) *$P(\cdot,t) = \mathbf{1}_{(-\infty,E(t))}(H(\cdot,t))$, or*

(b) *$P(\cdot,t) = P_m(\cdot,t)$ the eigenprojector corresponding to an isolated Bloch band $E_m(\cdot,t)$.*

Then

$$P(k,t) = \mathscr{R}_{\mathrm{f}}\, P(-k,t)\, \mathscr{R}_{\mathrm{f}}, \tag{6.1}$$

and the piezocurvature $\Theta = -\mathrm{i}\,\mathrm{tr}\,(P\,[\partial_t P,\, \nabla_k P])$ satisfies

$$\Theta(-k,t) = -\,\Theta(k,t). \tag{6.2}$$

Proof. The transformed Hamiltonian $\mathcal{Z}H(t)\mathcal{Z}^{-1}$ commutes with $\widetilde{\mathscr{R}}$, yielding a symmetry of the fibers, *i.e.*

$$H(k,t) = \mathscr{R}_{\mathrm{f}}\, H(-k,t)\, \mathscr{R}_{\mathrm{f}}. \tag{6.3}$$

In order to prove (6.1) one distinguish two cases.

Case (a). Since by assumption $E(t) \in \varrho\,(H(t))$, the resolvent set of $H(t)$, one has $E(t) \in \varrho\,(H(k,t))$ for a.e. $k \in Y^*$. By the continuity of the fibration the same holds true for every $k \in Y^*$. Then, by applying functional calculus to (6.3), one obtains (6.1).

Case (b). By the unitary equivalence (6.3) $E_m(k,t)$ is an eigenvalue of $H(-k,t)$. By the *continuity* of $k \mapsto E_m(k,t)$ and the *gap condition*, by starting from $k=0$ one concludes that $E_m(-k,t) = E_m(k,t)$ for any k, *i.e.* $E_m(k,t)$ is the eigenvalue corresponding to $P(-k,t)$. Let $f \in C_0^\infty(\mathbb{R})$ be the smoothed characteristic function of an interval containing $E_m(k,t) = E_m(-k,t)$ and no other point of $\sigma\left(H(k,t)\right) = \sigma\left(H(-k,t)\right)$. Then from (6.3) one gets

$$P(k,t) = f(H(k,t)) = \mathscr{R}_{\mathrm{f}} f(H(-k,t)) \mathscr{R}_{\mathrm{f}} = \mathscr{R}_{\mathrm{f}} P(-k,t) \mathscr{R}_{\mathrm{f}}.$$

In both cases from (6.1) one computes

$$\partial_{k_i} P(k,t) = -\,\mathscr{R}_{\mathrm{f}}\, \partial_{k_i} P(-k,t)\, \mathscr{R}_{\mathrm{f}}, \qquad \partial_t P(k,t) = \mathscr{R}_{\mathrm{f}}\, \partial_t P(-k,t)\, \mathscr{R}_{\mathrm{f}},$$

so that

$$\begin{aligned} \mathrm{i}\,\Theta(-k,t) &= -\operatorname{tr}\left(\mathscr{R}_{\mathrm{f}} P(k,t) \mathscr{R}_{\mathrm{f}}\, \mathscr{R}_{\mathrm{f}} [\partial_t P(k,t),\, \nabla_k P(k,t)] \mathscr{R}_{\mathrm{f}}\right) \\ &= -\operatorname{tr}\left(P(k,t)[\partial_t P(k,t),\, \nabla_k P(k,t)]\right) \\ &= -\,\mathrm{i}\,\Theta(k,t). \end{aligned}$$

□

We now turn to study the consequences of time-reversal symmetry. This symmetry is realized in $\mathcal{H} = L^2(\mathbb{R}^d)$ by the complex conjugation operator, *i.e.* by the operator

$$(\mathscr{C}\psi)(x) = \bar{\psi}(x), \qquad \psi \in L^2(\mathbb{R}^d).$$

By the Bloch Floquet transform we get that $\widetilde{\mathscr{C}} = \mathcal{Z}\mathscr{C}\mathcal{Z}^{-1}$ acts as

$$(\widetilde{\mathscr{C}}\psi)(k) = \mathscr{C}_{\mathrm{f}}\, \psi(-k), \qquad \psi \in L^2(Y_k^*) \otimes \mathcal{H}_{\mathrm{f}},$$

where $\mathscr{C}_{\mathrm{f}}$ is the complex conjugation operator in $\mathcal{H}_{\mathrm{f}}$.

Proposition 6.2 (Time-reversal symmetry). *Assume that the self-adjoint operator $H(t)$ commutes with $\mathscr{C}$ in $L^2(\mathbb{R}^d)$, and that $\mathcal{Z}H(t)\mathcal{Z}^{-1}$ is a* continuously *fibered operator. Let $P(\cdot,t)$ be as in Proposition 6.1. Then*

$$P(k,t) = \mathscr{C}_{\mathrm{f}}\, P(-k,t)\, \mathscr{C}_{\mathrm{f}}, \tag{6.4}$$

and the piezocurvature $\Theta = -\mathrm{i}\operatorname{tr}\left(P\,[\partial_t P,\, \nabla_k P]\right)$ satisfies

$$\Theta(-k,t) = \Theta(k,t). \tag{6.5}$$

The difference in sign between (6.5) and (6.2) is due to the fact that $\mathscr{C}_{\mathrm{f}}$ is an antilinear unitary operator, while $\mathscr{R}_{\mathrm{f}}$ is a linear one. Notice that the time dependence plays no role in the statement and in the proof of this proposition. Since the proof is very similar to the one of Proposition 6.1 we only point out some differences due to the fact that $\mathscr{C}_{\mathrm{f}}$ is an *antilinear* operator.

Proof. The starting point is again a symmetry of the fibers, namely

$$H(k,t) = \mathscr{C}_{\mathrm{f}} H(-k,t) \mathscr{C}_{\mathrm{f}}. \tag{6.6}$$

Case (a). One proceeds as in the previous proof, exploiting the fact that functional calculus is covariant with respect to complex conjugation, *i.e.* $f(\mathscr{C}_{\mathrm{f}}\, A\, \mathscr{C}_{\mathrm{f}}) = \mathscr{C}_{\mathrm{f}}\, f(A)\, \mathscr{C}_{\mathrm{f}}$ whenever A is self-adjoint and f is an admissible function.

Case (b). By assumption there exists $\varphi_m \in \mathcal{H}_{\mathrm{f}}$, $\varphi_m \neq 0$, such that

$$H(k,t)\varphi_m = E_m(k,t)\varphi_m$$

By complex conjugation one gets

$$E_m(k,t)\, \mathscr{C}_{\mathrm{f}} \varphi_m = \mathscr{C}_{\mathrm{f}} H(k,t) \varphi_m = \mathscr{C}_{\mathrm{f}} H(k,t) \mathscr{C}_{\mathrm{f}}\, \mathscr{C}_{\mathrm{f}} \varphi_m = H(-k,t)\, \mathscr{C}_{\mathrm{f}} \varphi_m,$$

which shows that $E_m(k,t)$ is an eigenvalue of $H(-k,t)$. Then one concludes the argument as in the previous Proposition.

In both cases by (6.4) one has

$$\partial_{k_i} P(k,t) = -\, \mathscr{C}_{\mathrm{f}}\, \partial_{k_i} P(-k,t)\, \mathscr{C}_{\mathrm{f}}, \quad \partial_t P(k,t) = \mathscr{C}_{\mathrm{f}}\, \partial_t P(-k,t)\, \mathscr{C}_{\mathrm{f}},$$

so that

$$\begin{aligned} \mathrm{i}\, \Theta(-k,t) = &\ -\mathrm{tr}\left(\mathscr{C}_{\mathrm{f}} P(k,t) \mathscr{C}_{\mathrm{f}}\, \mathscr{C}_{\mathrm{f}} [\partial_t P(k,t),\, \nabla_k P(k,t)] \mathscr{C}_{\mathrm{f}} \right) \\ = &\ \mathrm{tr}\left(P(k,t) [\partial_t P(k,t),\, \nabla_k P(k,t)] \right) \\ = &\ \mathrm{i}\, \Theta(k,t), \end{aligned}$$

where the minus sign disappears because of the *antilinearity* of $\mathscr{C}_{\mathrm{f}}$. □

6.2. **Geometric reinterpretation and electromagnetic analogy.** It is worthwhile to comment the relationship between the piezocurvature Θ and the *curvature of the Berry connection* Ω. The latter is the differential 2-form over $\mathbb{T}^*$ whose components are given by

$$\Omega_{j,l}(k,t) = -\mathrm{i}\, \mathrm{tr}\left(P(k,t) \left[\partial_j P(k,t),\, \partial_l P(k,t) \right] \right), \qquad j,l \in \{1, \ldots, d\}$$

where $\partial_j = \partial / \partial k_j$. As usual, this 2-form is identified with a vector field when convenient.[5] The importance of Ω is well-known. This curvature is indeed the main tool to compute the Chern class of the Bloch bundle *i.e.* the complex vector bundle over $\mathbb{T}^*$ whose fiber at the point $k \in \mathbb{T}^*$ is the subspace generate by a relevant set of Bloch functions. The vanishing of the mentioned Chern class is crucial in order to prove existence of localized Wannier functions [12, 11, 17] while in the magnetic case the analogous quantity represents the quantized transverse conductivity in the Integer Quantum Hall Effect [2].

[5] In dimension $d = 3$ one identifies the antisymmetric matrix $\Omega_{i,j}$ with the vector with components $\Omega_l = \sum_{i,j} \varepsilon_{lij} \Omega_{i,j}$, where ε_{ijl} is the totally antisymmetric symbol. Then Ω can be considered a vector field over $\mathbb{T}^3$. Similarly, for $d = 2$ the 2-form Ω is identified with a scalar function over $\mathbb{T}^2$.

In the following $P(k,t)$ can be interpreted in both the senses mentioned in Proposition 6.1. It is convenient to introduce Greek indexes $\mu,\nu \in \{0,1,\ldots,d\}$ and to pose $k_0 = t$ and $\partial_0 = \partial/\partial t$. The differential 2-form

$$\begin{aligned}\Xi(k,t) &:= \sum_{\mu,\nu=0}^{d} \Xi_{\mu,\nu}(k,t)\, dk_\mu \wedge dk_\nu \\ \Xi_{\mu,\nu}(k,t) &= -\,\mathrm{i}\,\mathrm{tr}\left(P(k,t)\left[\partial_\mu P(k,t),\, \partial_\nu P(k,t)\right]\right)\end{aligned}$$

over $M := \mathbb{T}^d \times \mathbb{R}$ represents the curvature of a connection on the *extended Bloch bundle*, *i.e.* the complex vector bundle over M whose fiber at (k,t) is the range of $P(k,t)$. More specifically Ξ is the curvature of the connection induced by the trivial connection in the trivial bundle (3.3), which is sometimes called *induced connection.* Equipped with this notation one has

$$\Omega_{j,l}(k,t) = \Xi_{j,l}(k,t) \quad \text{and} \quad \Theta_j(k,t) = \Xi_{j,0}(k,t),$$

where $j,l \in \{1,\ldots,d\}$.

The analogy with the electromagnetic field is striking: in this analogy Θ is identified with the electric field, while Ω with the magnetic field. The two fields combine into a tensor over "space-time" M. This analogy, rooted in the fact that both electromagnetism and the gauge theory of Bloch bands are gauge theories with structure group $U(1)$, is reinforced by an analysis of the transformation properties under time-reversal and space-reflection symmetry, which are summarized in the following self-explanatory table.

Quantity	**Time-reversal symmetry**	**Space-reflection symmetry**
$P(-k) =$	$\mathscr{C}_{\mathrm{f}}\, P(k)\, \mathscr{C}_{\mathrm{f}}$	$\mathscr{R}_{\mathrm{f}}\, P(k)\, \mathscr{R}_{\mathrm{f}}$
$\mathcal{A}(-k) =$	$+\mathcal{A}(k)$	$-\mathcal{A}(k)$
$\Omega(-k) =$	$-\Omega(k)$	$+\Omega(k)$
$\Theta(-k) =$	$+\Theta(k)$	$-\Theta(k)$

The table shows clearly that breaking of space-reflection symmetry is a necessary condition in order to have a non-zero piezoelectric current, while breaking of time-reversal symmetry is necessary in order to have a non-zero Chern class of the Bloch bundle over $\mathbb{T}^*$ and consequently a non-zero Hall conductance [2, 24].

We now specialize to case (b), namely $P(k,t) = P_m(k,t)$ is the eigenprojector corresponding to an isolated Bloch band. Then by introducing the Berry connection (1.13) and the geometric scalar potential (1.14), one obtains (locally in k) the following expressions,

$$\begin{aligned}\Omega_m &= \nabla \wedge \mathcal{A}_m & \Omega_{m\,j,l} &= \partial_j \mathcal{A}_{m\,l} - \partial_l \mathcal{A}_{m\,j} \\ \Theta_m &= -\partial_t \mathcal{A}_m - \nabla \phi_m & \Theta_{m\,j} &= -\partial_t \mathcal{A}_{m\,j} - \partial_j \phi_m.\end{aligned}$$

The latter formulae show again a strict analogy with the electromagnetic field, as noticed in [9].

Remark 6.3. (The case of a periodic deformation) The analysis of the previous sections, including formula (2.1), extends to the case of a periodic deformation of the crystal, *i.e.*

$$V_\Gamma(\cdot, t+T) = V_\Gamma(\cdot, t) \quad \forall\, t \in \mathbb{R},$$

for a suitable period T. In the periodic case the extended Bloch bundle ξ can be regarded as a vector bundle over $B_{\mathrm{per}} := \mathbb{T}^* \times \mathbb{T}^1_t$. Since B_{per} is a boundaryless manifold, the theory of characteristic classes applies to this case. In particular, focusing on $d = 3$ and choosing the third direction for sake of definiteness, the quantity

$$C_3(k_1, k_2) := \frac{1}{2\pi} \int_0^T \mathrm{d}t \int_{\mathbb{T}^1} \mathrm{d}k_3\, \Theta(k,t)_3,$$

where $k = (k_1, k_2, k_3)$ and $\mathbb{T}^1$ is the circle in the direction $\gamma_3^* \in \Gamma^*$, corresponds to the first Chern class of the restriction of ξ to the sub-manifold $\mathbb{T}^1_{k_3} \times \mathbb{T}^1_t \subset B_{\mathrm{per}}$, and as such is an integer. Since this integer depends continuously on (k_1, k_2), it is constant, *i.e.* $C_3(k_1, k_2) = c_3 \in \mathbb{Z}$.
On the other side, the same argument shows that the quantity

$$\tilde{C}_3(k_1, k_2) := \frac{1}{2\pi} \int_0^T \mathrm{d}t \int_{\mathbb{T}^1} \mathrm{d}k_3\, \Theta^\varepsilon_N(k,t)_3,$$

is also an integer, denoted as $\tilde{c_3}$. Thus from $\Theta^\varepsilon_N(k,t) = \Theta(k,t) + \mathcal{O}(\varepsilon)$ and $\varepsilon \ll 1$ one concludes that $\tilde{c_3} = c_3$, in agreement with the so-called *topological robustness* of the Chern class. In view of that, one gets

$$\begin{aligned} \Delta\mathbf{P}^\varepsilon &= -\frac{1}{(2\pi)^3} \int_0^T \mathrm{d}t \int_{\mathbb{T}^*} \mathrm{d}k\ \Theta^\varepsilon_N(k,t) + \mathcal{O}(\varepsilon^N) \\ &= -\frac{1}{(2\pi)^3} \int_0^T \mathrm{d}t \int_{\mathbb{T}^*} \mathrm{d}k\ \Theta(k,t) + \mathcal{O}(\varepsilon^N) \end{aligned}$$

which shows that the formula (2.3) holds true in the periodic case, even if $\dot{H}$ does not vanish at the boundaries of the time interval $[0, T]$. One concludes that

$$(\Delta\mathbf{P}^\varepsilon)_3 = -\frac{1}{(2\pi)^2} c_3 + \mathcal{O}(\varepsilon^N), \qquad c_3 \in \mathbb{Z}.$$

The macroscopic polarization is quantized up to errors smaller than any power of ε. As for $d = 1$, this fact has been pointed out by Thouless [26]. Notice that, in the adiabatic limit, the relative polarization is essentially a geometric quantity, namely the Chern class of a vector bundle. In particular it does not depend on the speed of the periodic deformation, *i.e.* $H(t)$ and $H(\lambda t)$, $\lambda \in \mathbb{R}$, lead to the same macroscopic polarization.

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