

Purely linear response of the quantum Hall current to space-adiabatic perturbations

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Abstract

Using recently developed tools from space-adiabatic perturbation theory, in particular the construction of a non-equilibrium almost-stationary state, we give a new proof that the Kubo formula for the Hall conductivity remains valid beyond the linear response regime. In particular, we prove that, in quantum Hall systems and Chern insulators, the transverse response current is quantized up to any order in the strength of the inducing electric field. The latter is introduced as a perturbation to a periodic, spectrally gapped equilibrium Hamiltonian by means of a linear potential; existing proofs of the exactness of Kubo formula rely instead on a time-dependent magnetic potential. The result applies to both continuum and discrete crystalline systems modelling the quantum (anomalous) Hall effect.

Keywords Linear response \cdot Quantum Hall effect \cdot Space-adiabatic perturbation theory \cdot Non-equilibrium almost-stationary state \cdot Chern marker

Mathematics Subject Classification $81Q15 \cdot 81Q20 \cdot 81V70$

1 Introduction and main results

The mathematical understanding of transport properties of quantum system is a fundamental question in the mathematical physics of condensed matter and still to date provides a stimulating challenge. The interest in this line of research has increased

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further after the discovery of "exotic" transport phenomena of topological origin, most notably the *quantum Hall effect*, where a 2-dimensional electron gas subject to a perpendicular magnetic field displays a transverse current in response to an inducing in-plane electric field of strength ε : at zero temperature, the conductivity for this transverse current can be computed by Kubo's formula at least in the linear response regime [26] and appears experimentally to be quantized (in appropriate physical units) to astounding precision [45]. More recently, a similar topological transport has been observed in *Chern insulators*, where time-reversal symmetry is broken by a different mechanism than an external magnetic field [7, 11, 12, 19]: this phenomenon is then called *quantum anomalous Hall effect*. New results are also pushing the study of topological transport and of the corresponding bulk-boundary correspondence to systems at positive temperature [14], but we will stick to the zero-temperature situation in the present paper.

The formula by Kubo expresses the transverse Hall current j as

$$j = \varepsilon \,\sigma_{\text{Hall}} + \mathcal{O}(\varepsilon^2),$$

where $\sigma_{\text{Hall}} \in (e^2/h) \mathbb{Z}$ is expressed in terms of equilibrium quantities (see below), involving in particular the Fermi projection Π_0 onto occupied energy levels; at positive temperature, this state would be replaced by a Fermi–Dirac distribution. Within the one-particle picture, as reviewed in [18], the quantization of the Hall conductivity has been understood mathematically by establishing its connection first with the *Chern number* of the Fermi projection from differential geometry [1], then with its non-commutative generalization, the *Connes–Chern character* (see [6] and references therein); the current physical literature [8, 10, 24] addresses this quantity under the name of (*local*) *Chern marker*. Recent mathematical efforts have managed to extend results in this direction also to the setting of electrons interacting on a lattice [4, 17, 20, 38, 44]. We refer the reader to the recent review [21] for further comments on the (mathematical) literature on the Kubo formula.

The topological nature of the Hall conductivity σ_{Hall} is believed to be responsible for its stability and robustness, making it *universal*, that is, independent of specific features of the model. Furthermore, its geometric origin is responsible also for the fact that the validity of the Kubo formula extends well beyond linear response: indeed, the conductivity associated with the transverse current of Hall systems is known to be equal to σ_{Hall} up to *arbitrarily high orders* in the strength ε of the perturbing electric field, that is,

$$j = \varepsilon \,\sigma_{\text{Hall}} + \mathcal{O}(\varepsilon^{\infty}). \tag{1.1}$$

The existing literature on this property was initiated by the heuristic *magnetic flux insertion argument* proposed by Laughlin in a cylindrical geometry [27], which was later elaborated in a rigorous way for many-body electron gases in the continuum [25] or discrete [5] setting. These proofs focus on a related quantity, namely the Hall *conductance*, defined as the (linear) response of the current intensity to the voltage drop: in two dimensions, this quantity agrees with the Hall *conductivity* σ_{Hall} defined above, see [2]. In the magnetic-flux-insertion argument, the inducing electric field

is modelled by a slowly varying time-dependent magnetic potential: this allows to follow time-adiabatically the insertion of this magnetic flux in the ground state. Klein and Seiler [25] then make use of the geometric interpretation of σ_{Hall} to conclude the validity of (the Hall-conductance analogue of) (1.1), at least up to averaging over time and over the inserted magnetic flux. Instead, Bachmann *et al.* [5] obtain an analogous statement (in the context of lattice spin systems with local interactions and observables) avoiding magnetic-flux averaging and the geometric argument, at the expense of exploiting the integrality of a certain Fredholm index related to the Hall conductance. Both approaches rely on the assumption that this magnetic flux insertion does not close the gap of the unperturbed Hamiltonian. More in general, in the standard time-adiabatic approach to charge transport [3, 4, 9, 15, 30, 38] the "global properties" of the unperturbed model are left invariant by the slowly varying perturbation: for example, the operator domain of the perturbed Hamiltonian is time-independent [3] and in infinite volume ergodicity is preserved by some form of covariance [9].

In this paper, we manage to prove the above-mentioned remarkable property of the Hall conductivity (Theorem 4.1) avoiding the magnetic flux insertion altogether and in particular the use of time-adiabatic perturbation theory. To model the equilibrium system, we employ the one-particle approximation and use a spectrally gapped (insulating) crystalline Hamiltonian H_0 ; this could be a discrete, tight-binding Hamiltonian, or a continuum (magnetic) Schrödinger-type operator. Contrary to the above-mentioned references, the external electric field will then be introduced by the addition of a linear potential to the equilibrium Hamiltonian, closer to how experimental setups for the quantum Hall effect were originally performed. More concretely, we will define the perturbed Hamiltonian as $H^{\varepsilon} = H_0 - \varepsilon Y$, where ε is a small parameter connected to the intensity of the electric field, which points in the y-direction. Notice in particular that the perturbation $-\varepsilon Y$ is an unbounded operator, even relatively to the unperturbed Hamiltonian H_0 , thus the domain of H^{ε} does depend on ε ; moreover, the perturbation breaks periodicity and closes the initial spectral gap of H_0 .

Our argument for the proof of (1.1) relies on two main tools:

- (1) by treating the linear electric potential as a *space-adiabatic perturbation* [41, 43] (see also [40] for earlier related works), we are able to construct a *non-equilibrium almost-stationary state* (NEASS), in the sense of [35, 44], which in the adiabatic regime well approximates the physical state of the system once the dynamical switching drives the Fermi projection out of equilibrium [36] (see the discussion at the end of Sect. 2);
- (2) the connection of the conductivity associated with the current flowing in the NEASS with its topological value σ_{Hall} is realized by a *Chern–Simons-like formula* (Proposition 4.4), similar to that used in [25].

By definition, the NEASS is unitarily conjugated to the equilibrium Fermi projection (see property (SA₁) below): this structure is reminiscent of the "magnetic gauge transformed projection" of [25], as well as of the "dressed ground state" of [5], with the main difference that the unitary conjugation is defined here by employing *spaceadiabatic* rather than time-adiabatic perturbation theory. The NEASS was constructed in [35] up to first order in ε in the same context that we will employ; using arguments from [44], we extend this construction to arbitrarily high orders in ε (Theorem 3.1), a result which is interesting in its own right.

Since we deal with extended systems, a prominent role is played by the *trace per unit volume* $\tau(\cdot)$, which is used to compute expectation values of extensive observables in (non-)equilibrium states: for example, the charge current which flows in the NEASS Π^{ε} equals (for carriers of unit charge)

$$\tau(\mathbf{i}[H_0, X] \Pi^{\varepsilon}),$$

and the quantized value of the Hall conductivity can be expressed (in appropriate physical units for which $e = \hbar = 1$) as

$$\sigma_{\text{Hall}} = \mathrm{i}\,\tau\left(\Pi_0\big[[\Pi_0, X], [\Pi_0, Y]\big]\right) \in \frac{1}{2\pi}\,\mathbb{Z},$$

if the electric field is applied, say, in direction y, and the transverse current is measured along direction x. To ensure the well-posedness of all traces per unit volume that need to be considered, we restrict ourselves to the setting of crystalline systems and *periodic* operators (that is, operators which commute with translations by crystalline shifts in a Bravais lattice) and introduce certain operator algebras of such operators (see Sect. 2.2). The heart of the proof is, however, of "algebraic" nature, and therefore, we believe that it may be generalized to apply to settings which also include ergodic disorder (at least under a mobility spectral gap assumption), in which the relevant operators satisfy only a covariance property when shifted by lattice translations (see, *e. g.* [9] for a framework of this type).

Finally, let us comment on the applicability of our result to spin transport. The discovery of topological insulators in the early 2000s stimulated the study of topological transport of spin, for example in the quantum spin Hall effect. When spin is a conserved quantity, namely when the spin-torque operator $i[H_0, S^z]$ vanishes, a spin current operator can be defined as $J^{z} = i[H_{0}, X] S^{z}$, and the response of this current to an external electric field can be also studied. As it is easily realized, this setting essentially amounts to two "copies" of a quantum Hall system (one corresponding to charge carriers with "up" spin, and one to those with "down" spin), and our result applies to this spin-filtered charge transport as well, leading to the quantization of the Hall conductivity in each spin channel separately. A much richer and mathematically more challenging situation would be to consider systems in which spin is not conserved, for example due to the presence of Rashba spin-orbit coupling in the model. With similar techniques to the ones presented in this paper, one can show that, as explained in Remark 4.5, even in this situation there is no generation of spin torque in the NEASS, namely that $\tau(i[H_0, S^z] \Pi^{\varepsilon}) = \mathcal{O}(\varepsilon^{\infty})$ [31]. Instead, while formulæ for the (appropriate generalization of) spin conductivity have been already investigated analytically [34, 35] and numerically [39] within linear response, the existence of possible power-law correction to these formulæ remains to be studied. We postpone this investigation to future work.

The paper is structured as follows: Section 2 details the class of models to which our result applies. Section 3 provides the construction of the NEASS to all orders in

 ε , generalizing the results of [35] beyond the linear regime. Section 4 finally contains the proof of our main result stating the validity of the Kubo formula for the Hall conductivity to arbitrarily high orders of ε . The Appendices contain, for the readers' convenience, some properties of the trace per unit volume and of the inverse Liouvillian of a gapped Hamiltonian, which are used throughout the paper.

2 Model and mathematical framework

2.1 Crystalline structures and periodic operators

The quantum systems we will be analyzing have a *crystalline structure*, meaning that their configuration space \mathcal{X} is invariant under translations by vectors in a Bravais lattice Γ . We will address both continuum and discrete models on the same footing: in *d*-dimensions, by a continuum configuration space we mean $\mathcal{X} = \mathbb{R}^d$, while a discrete configuration space is a discrete set of points. In both cases, it can be assumed that the Bravais lattice Γ is spanned over the integers by a basis $\{a_1, \ldots, a_d\} \subset \mathbb{R}^d$.

The Hilbert space for a quantum particle with N internal degrees of freedom (say, spin) will be

$$\mathcal{H}:=L^2(\mathcal{X})\otimes \mathbb{C}^N\simeq L^2(\mathcal{X},\mathbb{C}^N).$$

A prominent feature of this Hilbert space is the possibility to define (self-adjoint) *position operators*:

$$(X_j\psi)(x):=x_j\psi(x), \quad 1 \le j \le d.$$

The above definition of course makes sense only on a suitable (maximal) domain $\mathcal{D}(X_i) \subset \mathcal{H}$.

The crystalline structure of the configuration space is lifted to a symmetry of the one-particle Hilbert space, namely we assume that there is a unitary representation $T: \Gamma \rightarrow U(\mathcal{H}), \gamma \mapsto T_{\gamma}$, by *translation operators*. Let us note that, in the presence of uniform magnetic fields, these operators could be magnetic translations [46], assuming a commensurability condition on the magnetic flux per unit cell and the quantum of magnetic flux. These considerations are relevant for quantum Hall systems, which are included in our framework under the above-mentioned commensurability hypothesis. The case of non-commensurate magnetic fluxes could be treated by means of magnetic-covariant perturbation theory [40], which would require some slightly more involved analysis—see the discussion in Remark 3.2.

An operator A on \mathcal{H} is called *periodic* if $[A, T_{\gamma}] = 0$ for all $\gamma \in \Gamma$. As is wellknown, the analysis of periodic operators is simplified by the use of the *(magnetic) Bloch–Floquet–Zak representation* (see, e. g. [16] and references therein), which introduces the crystal momentum $k \in \mathbb{R}^d$ as a good quantum number. The *(magnetic) Bloch–Floquet–Zak transform* is initially defined on compactly supported functions $\psi \in C_0(\mathcal{X}, \mathbb{C}^N) \subset L^2(\mathcal{X}, \mathbb{C}^N)$ as

$$(\mathcal{U}_{\mathrm{BFZ}}\psi)(k, y) := \mathrm{e}^{-\mathrm{i}k \cdot y} \sum_{\gamma \in \Gamma} \mathrm{e}^{\mathrm{i}k \cdot \gamma} (T_{\gamma}\psi)(y) \quad \text{ for all } k \in \mathbb{R}^d, \ y \in \mathcal{X}.$$
(2.1)

For fixed $k \in \mathbb{R}^d$, the function $(\mathcal{U}_{BFZ}\psi)(k, \cdot)$ is periodic with respect to the translations operators; hence, it defines an element in the so-called fiber Hilbert space

$$\mathcal{H}_{\mathbf{f}} := \left\{ \phi \in L^2_{\text{loc}}(\mathcal{X}, \mathbb{C}^N) \mid T_{\gamma} \phi = \phi \text{ for all } \gamma \in \Gamma \right\}$$

which is equipped with the scalar product inducing the norm

$$\|\phi\|_{\mathcal{H}_{\mathrm{f}}}^{2} := \int_{\mathcal{C}_{1}} \mathrm{d}y \, |\phi(y)|^{2},$$

where C_1 is a fundamental cell for Γ (see (A.1)). The crystal momentum is effectively defined up to translations in the dual Bravais lattice Γ^* , consisting of those $\lambda \in \mathbb{R}^d$ such that $\lambda \cdot \gamma \in 2\pi\mathbb{Z}$ for all $\gamma \in \Gamma$: indeed,

$$(\mathcal{U}_{BFZ}\psi)(k+\gamma^*, y) = (\varrho_{\gamma^*}\mathcal{U}_{BFZ}\psi)(k, y) \text{ for all } \gamma^* \in \Gamma^*,$$

where $(\varrho_{\gamma^*}\varphi)(y):=e^{-i\gamma^*\cdot y}\varphi(y)$, and $\varrho\colon \Gamma^* \to \mathcal{U}(\mathcal{H}_f), \gamma^* \mapsto \varrho_{\gamma^*}$, defines a unitary representation. The map defined by (2.1) extends then to a unitary operator $\mathcal{U}_{BFZ}: \mathcal{H} \to \mathcal{H}_{\varrho}$, where $\mathcal{H}_{\varrho} \equiv L^2_{\varrho}(\mathbb{R}^d, \mathcal{H}_f)$ is the space of locally- L^2 , \mathcal{H}_f -valued, ϱ -equivariant functions on \mathbb{R}^d . Denoting by \mathbb{B}^d a fundamental cell for Γ^* , the inverse transformation $\mathcal{U}_{BFZ}^{-1}: \mathcal{H}_{\varrho} \to \mathcal{H}$ is explicitly given by

$$(\mathcal{U}_{\mathrm{BFZ}}^{-1}\varphi)(x) = \frac{1}{\left|\mathbb{B}^{d}\right|} \int_{\mathbb{B}^{d}} \mathrm{d}k \, \mathrm{e}^{\mathrm{i}k \cdot x} \varphi(k, x).$$

This transform is useful in the analysis of periodic operators as they become *covari*ant fibered operators on \mathcal{H}_{ρ} : upon the identification

$$\mathcal{H}_{\varrho} \equiv L^2_{\varrho}(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}}) \subset L^2(\mathbb{R}^d, \mathcal{H}_{\mathrm{f}}) \simeq \int_{\mathbb{R}^d}^{\oplus} \mathrm{d}k \, \mathcal{H}_{\mathrm{f}},$$

one has

$$\mathcal{U}_{\rm BFZ} A \, \mathcal{U}_{\rm BFZ}^{-1} = \int_{\mathbb{R}^d}^{\oplus} \mathrm{d}k \, A(k), \tag{2.2}$$

where each A(k) acts on \mathcal{H}_{f} and satisfies the covariance property

$$A(k + \gamma^*) = \varrho_{\gamma^*} A(k) \, \varrho_{\gamma^*}^{-1}, \quad \text{for all } k \in \mathbb{R}^d, \ \gamma^* \in \Gamma^*.$$

2.2 Operator algebras of periodic operators

Since the paper relies on the analysis of periodic operators, we will introduce in this section the necessary algebras of operators which have a smooth fiber in the Bloch–Floquet–Zak representation, in an appropriate sense. In the following, \mathcal{H}_1 and \mathcal{H}_2 will denote Hilbert subspaces of \mathcal{H}_f (possibly endowed with different norms than the subspace norm) which are left invariant by the action of all momentum-space translation operators ρ_{γ^*} , $\gamma^* \in \Gamma^*$. As we will specify in the next sections, in our applications such Hilbert spaces will be either \mathcal{H}_f itself, or the domain \mathcal{D}_f of the fiber unperturbed Hamiltonian (endowed with the graph norm of the latter).

Definition 2.1 Let $\mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$ denote the space of bounded linear operators from \mathcal{H}_1 to \mathcal{H}_2 , and $\mathcal{L}(\mathcal{H}_1):=\mathcal{L}(\mathcal{H}_1, \mathcal{H}_1)$. We define

$$\mathcal{P}(\mathcal{H}_1, \mathcal{H}_2) := \left\{ \text{ periodic operators } A \text{ with smooth fibration} \\ \mathbb{R}^d \to \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2), k \mapsto A(k) \right\}$$

equipped with the norm

$$\|A\|_{\mathcal{P}(\mathcal{H}_1,\mathcal{H}_2)} := \max_{k \in \mathbb{B}^d} \|A(k)\|_{\mathcal{L}(\mathcal{H}_1,\mathcal{H}_2)}.$$

We also set $\mathcal{P}(\mathcal{H}_1) := \mathcal{P}(\mathcal{H}_1, \mathcal{H}_1)$.

Since the Fréchet derivative follows the usual rules of differential calculus, we have that

- (1) $\mathcal{P}(\mathcal{H}_1, \mathcal{H}_2)$ is a linear space;
- (2) $\mathcal{P}(\mathcal{H}_1)$ is a normed algebra, as well as $\mathcal{P}(\mathcal{H}_1, \mathcal{H}_2)$ if $^1\mathcal{H}_2 \subset \mathcal{H}_1$;
- (3) if $\mathcal{H}_2 \subset \mathcal{H}_1$, then for $A \in \mathcal{P}(\mathcal{H}_2, \mathcal{H}_1)$ and $B \in \mathcal{P}(\mathcal{H}_1, \mathcal{H}_2)$ we have

$$AB \in \mathcal{P}(\mathcal{H}_1)$$
 with $||AB||_{\mathcal{P}(\mathcal{H}_1)} \leq ||A||_{\mathcal{P}(\mathcal{H}_2,\mathcal{H}_1)} ||B||_{\mathcal{P}(\mathcal{H}_1,\mathcal{H}_2)}$.

It is also useful to consider smooth functions in $\mathcal{H}_{\varrho} \equiv L^2_{\varrho}(\mathbb{R}^d, \mathcal{H}_f)$. As decay at infinity translates into regularity in *k* via the Bloch–Floquet–Zak transform, for example compactly supported functions of *x* are mapped by \mathcal{U}_{BFZ} to smooth functions of *k*.

Definition 2.2 We set

$$C_{\varrho}^{\infty}(\mathbb{R}^{d}, \mathcal{H}_{1}) := \left\{ \varphi \in \mathcal{H}_{\varrho} : \varphi(k, \cdot) \in \mathcal{H}_{1} \text{ for all } k \in \mathbb{R}^{d} \text{ and } \varphi : \mathbb{R}^{d} \to \mathcal{H}_{1} \text{ is smooth} \right\}.$$

This space of smooth functions, which is clearly dense in $L^2_{\varrho}(\mathbb{R}^d, \mathcal{H}_1)$, is particularly convenient to formulate the invariance of the operator algebras $\mathcal{P}(\mathcal{H}_1, \mathcal{H}_2)$ under the derivations given by the commutation with position operators, as detailed in the following statement. Its proof can be found in [35, Sect. 3].

¹ With this inclusion, we mean also that the inclusion $\mathcal{H}_2 \hookrightarrow \mathcal{H}_1$ is bounded as a map of normed spaces.

Lemma 2.3 Let $A \in \mathcal{P}(\mathcal{H}_1, \mathcal{H}_2)$. Then

$$[A, X_j] := [A, X_j] \Big|_{\mathcal{U}_{\mathrm{BFZ}}^{-1} C_{\varrho}^{\infty}(\mathbb{R}^d, \mathcal{H}_1)}$$

is in $\mathcal{P}(\mathcal{H}_1, \mathcal{H}_2)$, and

 $[A, X_j](k) \varphi(k) = -i\partial_{k_j} A(k) \varphi(k) \quad \text{for all } \varphi \in C_o^\infty(\mathbb{R}^d, \mathcal{H}_1).$

We conclude this section by recalling that the space $\mathcal{B}_{\infty}^{\tau}$ of bounded periodic operators is endowed with a trace-like functional, called the *trace per unit volume*, defined equivalently as

$$\tau(A) := \frac{1}{|\mathcal{C}_1|} \operatorname{Tr}_{\mathcal{H}} \left(\chi_{\mathcal{C}_1} A \chi_{\mathcal{C}_1} \right) \quad \text{or} \quad \tau(A) := \frac{1}{(2\pi)^d} \int_{\mathbb{B}^d} \mathrm{d}k \, \operatorname{Tr}_{\mathcal{H}_{\mathrm{f}}}(A(k)) \,,$$

whenever the right-hand sides make sense (see Proposition A.3). Here, χ_{C_1} is the multiplication operator times the characteristic function of the fundamental cell $C_1 \subset \mathcal{X}$. Periodic operators of *trace-per-unit-volume class* define the space \mathcal{B}_1^{τ} . As we will see shortly, the trace per unit volume is used to compute expectation values of extensive observables in the crystalline, periodic setting which we also employ. We refer the reader to Appendix A and to [35] for a list of the relevant properties of the trace per unit volume that will be repeatedly used in the paper.

2.3 The model

As stated in the Introduction, our goal is to investigate the response of a crystalline system to the application of an external constant electric field of small intensity. Consequently, a prominent role is played by the Hamiltonian H_0 of the system at equilibrium, before the electric field is applied and the response current is probed. Our assumptions on this unperturbed model, which coincide with those adopted in [35, Sect. 3], are stated below.

Assumption 2.4 We assume the following.

- (H₁) The Hamiltonian H_0 of the unperturbed system is a self-adjoint periodic operator on \mathcal{H} , bounded from below. Moreover, its fibers $H_0(k)$, defined in the Bloch–Floquet–Zak representation via (2.2), are self-adjoint operators with a common dense domain $\mathcal{D}_f \subset \mathcal{H}_f$. Finally, we assume that $H_0 \in \mathcal{P}(\mathcal{D}_f, \mathcal{H}_f)$, where hereinafter \mathcal{D}_f is understood to be equipped with the graph norm $\|\cdot\|_{\mathcal{D}_f}$ of the operator $H_0(0)$.
- (H₂) We assume the Fermi energy $\mu \in \mathbb{R}$ to lie in a spectral gap of H_0 . We denote by $\Pi_0 = \chi_{(-\infty,\mu)}(H_0)$ the corresponding spectral projector (Fermi projector). Finally, we assume that $\Pi_0 \in \mathcal{B}_1^{\tau}$.

² This assumption is equivalent to require that the fibration $k \mapsto \Pi_0(k)$ takes values in the finite-rank projections on \mathcal{H}_f . Indeed, in view of the fact that Π_0 is an orthogonal projection and the smoothness

The above assumptions are satisfied by a large class of physically relevant models, including tight-binding Hamiltonian of common use in condensed matter physics to model discrete systems, as well as Bloch–Landau operators (under mild regularity assumptions on the electro-magnetic potentials—see *e.g.* [37, Sect. 3]) used as continuum models for crystalline systems.

We list below a number of relevant properties which can be deduced from the above Assumption, in combination with Lemma 2.3, and which will be used repeatedly throughout the paper. As before, we refer the reader to [35, Sect. 3] for a proof.

Proposition 2.5 Under Assumption 2.4, we have that

- (*i*) for every $z \in \rho(H_0)$ the resolvent operator $(H_0 z\mathbb{1})^{-1}$ lies in $\mathcal{P}(\mathcal{H}_f, \mathcal{D}_f)$, and consequently Π_0 is in $\mathcal{P}(\mathcal{H}_f, \mathcal{D}_f)$ as well;
- (ii) all iterated commutators of H_0 with position operators lie in $\mathcal{P}(\mathcal{D}_f, \mathcal{H}_f)$, while all iterated commutators of Π_0 with position operators lie in $\mathcal{P}(\mathcal{H}_f, \mathcal{D}_f)$.

Having specified the conditions on the model at equilibrium, we drive the system out of equilibrium by introducing an external constant electric field. We choose the direction of this field to be along a preferred coordinate, say *y*. The perturbation will then be modelled space-adiabatically by adding a linear potential to the unperturbed Hamiltonian, namely

$$H^{\varepsilon} := H_0 - \varepsilon Y \,, \tag{2.3}$$

where $\varepsilon \in [0, 1]$ and Y denotes the multiplication operator by the coordinate function y.

We will be interested in measuring the response to this perturbation of a (possibly different) coordinate of the charge current operator, say along x: assuming charge carriers of unit charge,

$$J:=i[H_0, X],$$
 (2.4)

where *X* denotes the multiplication operator by *x*. This response will be computed in an appropriate out-of-equilibrium state, called *non-equilibrium almost-stationary state* (NEASS) in [44], that will be constructed in the next section. Conventionally, a candidate non-equilibrium state would be identified via time-adiabatic perturbation theory, as follows. Consider the time-dependent perturbed Hamiltonian

$$H^{\varepsilon,\eta}(t) := H_0 - \varepsilon f(\eta t)Y, \quad \text{for } t \in \mathbb{R}, \ 0 < \eta \ll 1,$$
(2.5)

where f is a switching function, that is $f : \mathbb{R} \to [0, 1]$ is a smooth map such that f(s) = 0 for $s \leq -1$ and f(s) = 1 for $s \geq 0$, and η plays the role of a timeadiabatic parameter. A natural choice for the non-equilibrium state is the solution of

assumption (H₁), it follows that the dimension m(k) of the range of $\Pi_0(k)$ is independent of k, i.e., $m(k) = m \in \mathbb{N} \cup \{+\infty\}$ for all $k \in \mathbb{B}^d$. Therefore, by virtue of Proposition A.3(iii) $\Pi_0 \in \mathcal{B}_1^{\tau}$ is equivalent to $m < \infty$.

the Cauchy problem associated with $H^{\varepsilon,\eta}(t)$ at t = 0 (or any nonnegative time, when the perturbation is fully on), *i.e.* $\rho^{\varepsilon,\eta} := \rho^{\varepsilon,\eta}(0)$ where $\rho^{\varepsilon,\eta}(t)$ solves

$$\begin{cases} i \frac{d}{dt} \rho^{\varepsilon,\eta}(t) = [H^{\varepsilon,\eta}(t), \rho^{\varepsilon,\eta}(t)] \\ \rho^{\varepsilon,\eta}(-\infty) = \Pi_0. \end{cases}$$
(2.6)

In order to compute the current response $\tau(J \rho^{\varepsilon,\eta})$ without the need for a timeadiabatic limit $\eta \to 0^+$, we will exploit the fact that $\rho^{\varepsilon,\eta}$ is well-approximated by an η -independent projection, namely the NEASS. More precisely, one can prove [36] that for all times $t \ge 0$ and any nonzero $n \in \mathbb{N}$

$$\left|\tau(A\,\rho^{\varepsilon,\eta}(t)) - \tau(A\,\Pi_n^{\varepsilon})\right| = \mathcal{O}(\varepsilon^{n+1}),\tag{2.7}$$

where Π_n^{ε} is the NEASS constructed in the next section. Inequality (2.7) holds for *suit-able* observables *A* (*e. g.* the charge current operator) uniformly on bounded intervals in (macroscopic) time and uniformly in an appropriate time-scale interval for η , which in general depends on the perturbation intensity ε . The same inequality was already shown in the context of interacting fermions on finite lattices in [44, Proposition 3.2, Theorem 5.1], and remains valid in the thermodynamic limit under a uniform spectral gap assumption [22] or under a spectral gap hypothesis only in the bulk [23]. For a more detailed comparison between the standard time-adiabatic approach to electronic transport and the NEASS paradigm, see [31, Sects. II.A & II.B].

3 Construction of the NEASS to all orders

In this section, we generalize the construction of the *non-equilibrium almost-stationary state* (NEASS), realized up to the first order in ε in [35, Section 4], to all orders, following the construction performed in the context of interacting models on lattices by [44] (see [4, 38] for related statements in time-dependent adiabatic perturbation theory). For every $n \in \mathbb{N}$ the NEASS, denoted by $\prod_{n=1}^{\varepsilon}$, is determined uniquely (up to terms of order $\mathcal{O}(\varepsilon^{n+1})$) by the following two properties:

(SA₁) $\Pi_n^{\varepsilon} = e^{-i\varepsilon S_n^{\varepsilon}} \Pi_0 e^{i\varepsilon S_n^{\varepsilon}}$ for some bounded, periodic and self-adjoint operator S_n^{ε} ;

(SA₂) Π_n^{ε} almost commutes with the Hamiltonian H^{ε} , namely $[H^{\varepsilon}, \Pi_n^{\varepsilon}] = \mathcal{O}(\varepsilon^{n+1})$.

Here $\mathcal{O}(\varepsilon^{n+1})$ is understood in the sense of the operator norm.

Theorem 3.1 Consider the Hamiltonian $H^{\varepsilon} = H_0 - \varepsilon Y$ where H_0 satisfies Assumption 2.4. Then, there exists a sequence $\{A_j\}_{j \in \mathbb{N}} \subset \mathcal{P}(\mathcal{H}_f, \mathcal{D}_f)$ such that, setting for any $n \in \mathbb{N}$

$$S_0^{\varepsilon} := 0 \quad and \quad S_n^{\varepsilon} := \sum_{j=1}^n \varepsilon^{j-1} A_j \in \mathcal{P}(\mathcal{H}_{\mathrm{f}}, \mathcal{D}_{\mathrm{f}}) \text{ for } n \ge 1,$$
 (3.1)

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we have that

$$\Pi_n^{\varepsilon} := \mathrm{e}^{\mathrm{i}\varepsilon \mathcal{S}_n^{\varepsilon}} \Pi_0 \, \mathrm{e}^{-\mathrm{i}\varepsilon \mathcal{S}_n^{\varepsilon}} \quad satisfies \quad [H^{\varepsilon}, \Pi_n^{\varepsilon}] = \varepsilon^{n+1}[R_n^{\varepsilon}, \Pi_n^{\varepsilon}] \tag{3.2}$$

where the map $[0, 1] \ni \varepsilon \mapsto R_n^{\varepsilon} \in \mathcal{P}(\mathcal{H}_f) \subset \mathcal{B}_{\infty}^{\tau}$ is bounded.

Proof We start by computing

$$[H^{\varepsilon}, \Pi_{n}^{\varepsilon}] = e^{i\varepsilon S_{n}^{\varepsilon}} \left[e^{-i\varepsilon S_{n}^{\varepsilon}} H_{0} e^{i\varepsilon S_{n}^{\varepsilon}} - \varepsilon e^{-i\varepsilon S_{n}^{\varepsilon}} Y e^{i\varepsilon S_{n}^{\varepsilon}}, \Pi_{0} \right] e^{-i\varepsilon S_{n}^{\varepsilon}}$$

Hence, it suffices to choose the operators A_j in such a way that there exists R_n^{ε} uniformly bounded in ε with

$$\left[e^{-i\varepsilon\mathcal{S}_{n}^{\varepsilon}}H_{0}e^{i\varepsilon\mathcal{S}_{n}^{\varepsilon}}-\varepsilon e^{-i\varepsilon\mathcal{S}_{n}^{\varepsilon}}Ye^{i\varepsilon\mathcal{S}_{n}^{\varepsilon}},\Pi_{0}\right]=\varepsilon^{n+1}\left[e^{-i\varepsilon\mathcal{S}_{n}^{\varepsilon}}R_{n}^{\varepsilon}e^{i\varepsilon\mathcal{S}_{n}^{\varepsilon}},\Pi_{0}\right].$$
(3.3)

Consider the Taylor expansion in λ near $\lambda_0 = 0$ of the expression

$$e^{-i\lambda S_n^{\varepsilon}}Be^{i\lambda S_n^{\varepsilon}}$$

Evaluating such expansion at $\lambda = \varepsilon$, one obtains for some $\tilde{\varepsilon} \in [0, \varepsilon]$

$$e^{-i\varepsilon S_n^{\varepsilon}} B e^{i\varepsilon S_n^{\varepsilon}} = \sum_{k=0}^n \frac{\varepsilon^k}{k!} \mathscr{L}_{S_n^{\varepsilon}}^k(B) + \frac{\varepsilon^{n+1}}{(n+1)!} e^{-i\widetilde{\varepsilon} S_n^{\varepsilon}} \mathscr{L}_{S_n^{\varepsilon}}^{n+1}(B) e^{i\widetilde{\varepsilon} S_n^{\varepsilon}}$$
$$=: \sum_{j=0}^n \varepsilon^j B_j + \varepsilon^{n+1} B_{n+1}(\varepsilon).$$

On the first line, we use the notation $\mathscr{L}_A(B) := -i[A, B]$, we denoted by $\mathscr{L}_A^k(B)$ the *k* nested commutators [-iA, [..., [-iA, [-iA, B]]...]] for $k \ge 1$ and we set $\mathscr{L}_A^0(B) := B$. On the second line, we collected in B_j all the terms of order ε^j , $0 \le j \le n$, coming from the power expansion of S_n^{ε} as in the statement, while $B_{n+1}(\varepsilon)$ contains contributions from higher-order powers of ε and still defines a uniformly bounded function of ε . In particular, each of these coefficients is expressed as nested commutators involving (possibly different) A_{μ} 's with B: for example

$$B_0 = B$$
, $B_1 = -i[A_1, B]$, $B_2 = -\frac{1}{2}[A_1, [A_1, B]] - i[A_2, B]$.

We apply the expansion above to $B = H_0$ and a similar expansion, up to order n-1, to B = Y. We will therefore denote the corresponding coefficients by $H_{0,j}$ and Y_j , respectively. Notice that the presence of an extra factor of ε in the perturbation $H^{\varepsilon} - H_0 = -\varepsilon Y$ shifts the indices of the coefficients Y_j by one in the following equations.

Plugging all the expansions into (3.3) yields

$$\sum_{j=1}^{n} \varepsilon^{j} \left[H_{0,j} - Y_{j-1}, \Pi_{0} \right] + \varepsilon^{n+1} \left[H_{0,n+1}(\varepsilon) - Y_{n}(\varepsilon), \Pi_{0} \right]$$
$$= \varepsilon^{n+1} \left[e^{-i\varepsilon S_{n}^{\varepsilon}} R_{n}^{\varepsilon} e^{i\varepsilon S_{n}^{\varepsilon}}, \Pi_{0} \right]$$
(3.4)

(notice that the sum on the left-hand side starts from j = 1 as for j = 0 we get $[H_{0,0}, \Pi_0] = [H_0, \Pi_0] = 0$). Thus, it suffices to determine A_1, \ldots, A_n in such a way that for all $j \in \{1, \ldots, n\}$

$$0 = \left[H_{0,j} - Y_{j-1}, \Pi_0 \right].$$
(3.5)

To this end, it is convenient to notice that

$$H_{0,j} = \mathscr{L}_{A_j}(H_0) + L_{j-1} = -\mathscr{L}_{H_0}(A_j) + L_{j-1}$$

where L_{j-1} involves commutators of H_0 with the operators A_{μ} with $\mu < j$. Therefore, if we assume that A_1, \ldots, A_{j-1} have been already determined, then L_{j-1} is given and only A_j is still unknown in the above equality: this suggests to determine A_1, \ldots, A_n recursively.

Let us first start then by determining A_1 from (3.5). Since $L_0 = 0$ and $Y_0 = Y$, the equation for A_1 reads

$$0 = [-\mathscr{L}_{H_0}(A_1) - Y, \Pi_0] \implies [\mathscr{L}_{H_0}(A_1), \Pi_0] = \mathscr{L}_{H_0}([A_1, \Pi_0]) = -[Y, \Pi_0].$$

Notice that the operator $[Y, \Pi_0]$ is off-diagonal with respect to the decomposition $\mathcal{H} = \operatorname{Ran} \Pi_0 \oplus (\operatorname{Ran} \Pi_0)^{\perp}$, i.e.,

$$[Y, \Pi_0] = [Y, \Pi_0]^{\text{OD}} \text{ where } T^{\text{OD}} := \Pi_0 T \Pi_0^{\perp} + \Pi_0^{\perp} T \Pi_0 = \left[[T, \Pi_0], \Pi_0 \right]$$

(we denote by $\Pi_0^{\perp} := \mathbb{1} - \Pi_0$ the orthogonal projection on $(\operatorname{Ran} \Pi_0)^{\perp}$). As is well-known (see Appendix B) the Liouvillian \mathscr{L}_{H_0} is invertible on such operators, yielding

$$[A_1, \Pi_0] = \left[A_1^{\text{OD}}, \Pi_0\right] = \mathscr{L}_{H_0}^{-1}(-[Y, \Pi_0]).$$

Taking a further commutator of both sides with Π_0 , we conclude

$$A_1^{\text{OD}} = \left[\left[A_1^{\text{OD}}, \Pi_0 \right], \Pi_0 \right] = \left[\mathscr{L}_{H_0}^{-1}(-[Y, \Pi_0]), \Pi_0 \right] = -\mathscr{L}_{H_0}^{-1}(Y^{\text{OD}}).$$

The above considerations hence determine uniquely the off-diagonal part of A_1 ; we may then choose to set

$$A_1^{\rm D}:=0.$$

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For $1 < j \le n$, we are then required to solve

$$0 = -\mathscr{L}_{H_0} \left(\begin{bmatrix} A_j, \Pi_0 \end{bmatrix} \right) + \begin{bmatrix} L_{j-1}, \Pi_0 \end{bmatrix} - \begin{bmatrix} Y_{j-1}, \Pi_0 \end{bmatrix}$$
$$\implies \begin{bmatrix} A_j, \Pi_0 \end{bmatrix} = \mathscr{L}_{H_0}^{-1} \left(\begin{bmatrix} L_{j-1}, \Pi_0 \end{bmatrix} - \begin{bmatrix} Y_{j-1}, \Pi_0 \end{bmatrix} \right)$$

or, arguing as above,

$$A_j^{\text{OD}} = \mathscr{L}_{H_0}^{-1} (D_{j-1}) \text{ where } D_{j-1} := (L_{j-1} - Y_{j-1})^{\text{OD}}$$

Observe that L_{j-1} and Y_{j-1} are determined by the previously computed A_1, \ldots, A_{j-1} . Once again, we choose A_j to be purely off-diagonal, that is,

$$A_{i}^{D} := 0.$$

In conclusion, we have determined

$$\mathcal{S}_{n}^{\varepsilon} = \sum_{j=1}^{n} \varepsilon^{j-1} A_{j} = \mathscr{L}_{H_{0}}^{-1} \left(\sum_{\ell=0}^{n-1} \varepsilon^{\ell} D_{\ell} \right) \in \mathcal{P}(\mathcal{H}_{\mathrm{f}}, \mathcal{D}_{\mathrm{f}}).$$

As each A_j and then S_n^{ε} are inverse Liouvillians of off-diagonal operators in $\mathcal{P}(\mathcal{H}_f)$ by virtue of Lemma 2.3, they are naturally in $\mathcal{P}(\mathcal{H}_f, \mathcal{D}_f)$ as claimed (see Proposition B.1). With this definition of S_n^{ε} , it follows by construction that (3.4) will be satisfied if we set

$$R_n^{\varepsilon} := \mathrm{e}^{\mathrm{i}\varepsilon \mathcal{S}_n^{\varepsilon}} \left(H_{0,n+1}(\varepsilon) - Y_n(\varepsilon) \right) \mathrm{e}^{-\mathrm{i}\varepsilon \mathcal{S}_n^{\varepsilon}}.$$

Clearly, this remainder term is uniformly bounded as a function of ε with values in $\mathcal{P}(\mathcal{H}_f)$ in view of the previous discussion on $H_{0,n+1}(\varepsilon)$ and $Y_n(\varepsilon)$.

Remark 3.2 Clearly the expression $\Pi_n^{\varepsilon} = e^{i\varepsilon S_n^{\varepsilon}} \Pi_0 e^{-i\varepsilon S_n^{\varepsilon}}$ can be used also to obtain a Taylor expansion for the NEASS in powers of ε :

$$\Pi_n^{\varepsilon} = \Pi_0 + \varepsilon \,\Pi_1 + \varepsilon^2 \,\Pi_2 + \dots + \varepsilon^n \,\Pi_n + \varepsilon^{n+1} \Pi_{\text{reminder}}(\varepsilon). \tag{3.6}$$

The coefficients Π_{ℓ} in the above expansion are computable in terms of the A_j 's in the statement of Theorem 3.1: more specifically, Π_{ℓ} will be determined from A_1, \ldots, A_{ℓ} . As these A_j 's are determined inductively as in the proof (that is, A_1, \ldots, A_{ℓ} determine $A_{\ell+1}$), it is also clear that the above Taylor expansions for the NEASS's Π_n^{ε} and Π_{n+1}^{ε} coincide up to order ε^n . Explicit expressions for the coefficients in this Taylor expansion are in any case not needed for the proof of our main Theorem 4.1 in the next section.

The order-by-order construction of Π_n^{ε} as an expansion in powers of ε as in (3.6), or rather the construction of an "almost-invariant subspace" for the perturbed dynamics which is associated with a projection Π^{ε} expressed as an asymptotic power series in ε , is at the heart of the original approach to space-adiabatic perturbation theory [40, 41,

43]. It is worth noting that the coefficients of the Taylor expansion (3.6) coincide with what one would obtain from this order-by-order construction. The almost-invariant subspace can be produced also under weaker hypotheses than the ones we formulate in Assumption 2.4: in particular, Nenciu [40, Theorem 4.1] showed that, aside from certain typical domain specifications that ensure the self-adjointness of H^{ε} and from the spectral gap condition, it is sufficient to assume that the operator-valued map $t \mapsto e^{iYt} (H_0 - i\mathbb{1})^{-1} e^{-iYt}$ is norm-differentiable sufficiently many times. This condition amounts to the boundedness of iterated commutators of (the resolvent of) H_0 and Y: in view of Lemma 2.3 and of Proposition 2.5, in the periodic setting this is essentially equivalent to our Assumption 2.4 on the unperturbed Hamiltonian, which is instead formulated as a smoothness condition of its Bloch-Floquet fibers with respect to the crystal momentum. Nenciu's assumption is more general and can be verified in a larger class of models, which could include e.g. periodicity-breaking disordered potentials or a constant magnetic field of incommensurate flux per unit cell. To simplify our analysis and to make a closer connection to the recent literature on the NEASS [35, 38, 44], we decided, however, to concentrate only on translationally invariant models falling in the operator algebras described in Section 2.2, leaving to future investigations the technical details needed to adapt our proofs to more general settings.

We conclude this section with some immediate consequences from the previous theorem, which will be used in the next section.

Corollary 3.3 Consider the Hamiltonian $H^{\varepsilon} = H_0 - \varepsilon Y$ where H_0 satisfies Assumption 2.4. Then we have that for every $n \in \mathbb{N}$

- (*i*) the operator $(\Pi_n^{\varepsilon})^{\perp} H^{\varepsilon} \Pi_n^{\varepsilon} = \varepsilon^{n+1} (\Pi_n^{\varepsilon})^{\perp} R_n^{\varepsilon} \Pi_n^{\varepsilon}$ lies in \mathcal{B}_1^{τ} and the map $[0, 1] \ni \varepsilon \mapsto (\Pi_n^{\varepsilon})^{\perp} H^{\varepsilon} \Pi_n^{\varepsilon} \in \mathcal{B}_1^{\tau}$ is bounded;
- (ii) for S_n^{ε} as in (3.1), the operator $e^{i\varepsilon S_n^{\varepsilon}} \mathbb{1}$ lies in $\mathcal{P}(\mathcal{H}_f, \mathcal{D}_f)$ and the map $[0, 1] \ni \varepsilon \mapsto e^{i\varepsilon S_n^{\varepsilon}} \mathbb{1} \in \mathcal{P}(\mathcal{H}_f, \mathcal{D}_f)$ is bounded;
- (iii) the NEASS operator Π_n^{ε} lies in $\mathcal{P}(\mathcal{H}_f, \mathcal{D}_f)$ and the map $[0, 1] \ni \varepsilon \mapsto [X, \Pi_n^{\varepsilon}] \in \mathcal{P}(\mathcal{H}_f)$ is bounded.
- **Proof** (i) The statement is an immediate consequence of (3.2), the fact that $\Pi_n^{\varepsilon} (\Pi_n^{\varepsilon})^{\perp} = (\Pi_n^{\varepsilon})^{\perp} \Pi_n^{\varepsilon} = 0$, and the fact that Π_n^{ε} is unitarily equivalent to Π_0 , implying that it is a projection in \mathcal{B}_1^{τ} by hypothesis (H₂).
- (*ii*) In view of (3.1) $S_n^{\varepsilon} \in \mathcal{P}(\mathcal{H}_f, \mathcal{D}_f)$, thus [35, Lemma 6.4] implies the thesis.
- (*iii*) By using Proposition 2.5(ii), [35, Lemma 6.4] and the Leibniz rule, we obtain that $[X, \Pi_n^{\varepsilon}] \in \mathcal{P}(\mathcal{H}_f)$ and its norm is bounded uniformly in ε .

 \Box

4 Validity of the Kubo formula beyond the linear regime

We are finally able to state our main result.

Theorem 4.1 Consider the Hamiltonian $H^{\varepsilon} = H_0 - \varepsilon Y$ where H_0 satisfies Assumption 2.4. Then for every $n \in \mathbb{N}$ we have that

$$\tau(J \Pi_n^{\varepsilon}) = \varepsilon \,\sigma_{\text{Hall}} + \mathcal{O}(\varepsilon^{n+1}),$$

where J is the charge current operator in (2.4), the NEASS Π_n^{ε} is as in the statement of Theorem 3.1, and

$$\sigma_{\text{Hall}}:=i\tau(\Pi_0[[\Pi_0, X], [\Pi_0, Y]]).$$

The above Theorem states that the conductivity associated with the response of the current operator J is given by the Hall conductivity σ_{Hall} , a quantity which is defined only through the equilibrium Fermi projection Π_0 and which emerges at the linear level (Kubo formula), up to orders which are arbitrarily high in the strength of the perturbing electric field. The result thus establishes the validity of the Kubo formula for this conductivity also beyond linear response.

The proof of the above theorem relies on a number of intermediate steps, which we detail first.

4.1 A useful proposition

As a first tool to be used in the argument for the main Theorem 4.1, we prove the following

Proposition 4.2 Let P be a projection on \mathcal{H} such that $P \in \mathcal{P}(\mathcal{H}_{f}) \cap \mathcal{B}_{1}^{\tau}$. Assume that the operator A is such that $PAP \in \mathcal{P}(\mathcal{H}_{f})$. Then for all $j \in \{1, ..., d\}$ the trace per unit volume of the commutator $[PAP, PX_{j}P]$ is well-defined and

$$\tau([PAP, PX_iP]) = 0.$$

Proof We observe that

$$[PAP, PX_{i}P] = [PAP, X_{i}] - [PAP, X_{i}^{OD}]$$

where X_j^{OD} refers to the off-diagonal decomposition of the operator X_j with respect to the projection P, and the equality is first established on the dense subspace $\mathcal{U}_{\text{BFZ}}^{-1}C_{\varrho}^{\infty}(\mathbb{R}^d, \mathcal{H}_f)$. Proposition A.3(iv) implies that the first summand on the righthand side has vanishing trace per unit volume, since $PAP \in \mathcal{P}(\mathcal{H}_f) \cap \mathcal{B}_1^{\tau}$. On the other hand, the second summand is \mathcal{B}_1^{τ} in view of the hypothesis that $P \in \mathcal{P}(\mathcal{H}_f) \cap \mathcal{B}_1^{\tau}$ (see Lemma 2.3); invoking Lemma A.2, we conclude that its trace per unit volume vanishes.

Remark 4.3 Observe that the above Proposition does *not* apply to the operator $A = X_i$, $i \neq j$; indeed (compare *e. g.* [33, Eq. (2.15)])

$$[PX_iP, PX_jP] = P[[P, X_i], [P, X_j]]P,$$

where the equality is first established on $\mathcal{U}_{BFZ}^{-1}C_{\varrho}^{\infty}(\mathbb{R}^d, \mathcal{H}_f)$. Therefore, the trace per unit volume $\tau([PX_iP, PX_jP])$ equals (up to a factor $2\pi i$) the Chern marker of the projection *P*, which may very well be nonzero (cf. the discussion in the Introduction).

As we saw in the statement of the main result, the Chern marker of the Fermi projection Π_0 defines the linear response coefficient σ_{Hall} . It is worth mentioning that, in the present context of periodic operators, the (non-)vanishing of the Chern marker has been linked to the (non-)existence of localized orthogonal *Wannier functions* spanning the Fermi projection Π_0 [13, 32, 37]. In a more general setting, where periodicity is broken, one can still define a generalized notion of Wannier basis for an isolated spectral island, but the relation of its existence with the Chern marker remains to be fully understood. In fact, while the existence of a generalized Wannier basis (with suitable localization) has been shown to imply the vanishing of the Chern marker (see [28, 33]), the converse implication [29] remains a challenging and interesting line of research.

4.2 Chern–Simons formula

Following the previous Remark, we prove an analogue of the *Chern–Simons formula*, well rooted in differential geometry and bundle theory, which was exploited in [25] in a context similar to ours. There, the Hall conductance is related to the *Berry curvature* of an adiabatic spectral projection, viewed as a differential 2-form on the torus of magnetic fluxes: the Chern–Simons formula then describes how the Berry curvature changes by an exact form under unitary conjugation of the associated projection, and therefore, its integral over the torus of fluxes is left unchanged under such transformations. Our Chern–Simons formula similarly establishes the invariance of the Chern marker of a projection under suitable unitary conjugations.

Proposition 4.4 (Chern–Simons formula). Let $P \in \mathcal{P}(\mathcal{H}_f) \cap \mathcal{B}_1^\tau$ be a projection and $U \in \mathcal{P}(\mathcal{H}_f)$ be unitary. Define $P_U := UPU^{-1}$. Then

$$\tau([P_U X_i P_U, P_U X_j P_U]) = \tau([P X_i P, P X_j P]).$$

Proof Write

$$U^{-1}[P_U X_i P_U, P_U X_j P_U]U$$

= $[PU^{-1}X_i UP, PU^{-1}X_j UP]$
= $[PX_i P, PX_j P] + [PU^{-1}[X_i, U]P, PX_j P]$
+ $[PX_i P, PU^{-1}[X_j, U]P] + [PU^{-1}[X_i, U]P, PU^{-1}[X_j, U]P].$

Notice now that, with the standing assumptions, the operators $U^{-1}[X_i, U]$ and $U^{-1}[X_j, U]$ are in $\mathcal{P}(\mathcal{H}_f)$ by virtue of Lemma 2.3. Using Proposition 4.2 and Lemma A.2, the conclusion follows.

4.3 Proof of theorem 4.1

First of all, notice that by the very definition of the current operator J in (2.4) and the construction of the NEASS $\prod_{n=1}^{\varepsilon}$ in Theorem 3.1

$$J \Pi_n^{\varepsilon} = \mathbf{i}[H_0, X] \left(\mathbf{e}^{\mathbf{i}\varepsilon \mathcal{S}_n^{\varepsilon}} - \mathbb{1} \right) \Pi_0 \mathbf{e}^{-\mathbf{i}\varepsilon \mathcal{S}_n^{\varepsilon}} + \mathbf{i}[H_0, X] \Pi_0 \mathbf{e}^{-\mathbf{i}\varepsilon \mathcal{S}_n^{\varepsilon}},$$

where each summand on the right-hand side is in \mathcal{B}_1^{τ} . Indeed, for the first summand observe that

$$\begin{split} & [H_0, X] \cdot \left(e^{i\varepsilon \mathcal{S}_n^{\varepsilon}} - \mathbb{1} \right) \cdot \Pi_0 \cdot e^{-i\varepsilon \mathcal{S}_n^{\varepsilon}} \in \mathcal{P}(\mathcal{D}_f, \mathcal{H}_f) \cdot \mathcal{P}(\mathcal{H}_f, \mathcal{D}_f) \cdot \mathcal{B}_1^{\tau} \cdot \mathcal{P}(\mathcal{H}_f) \\ & \subset \mathcal{P}(\mathcal{H}_f) \cap \mathcal{B}_1^{\tau}, \end{split}$$

by applying Proposition 2.5(ii), Corollary 3.3(ii), and hypothesis (H₂). Similarly, for the second summand note that

$$[H_0, X] \cdot \Pi_0 \cdot \Pi_0 e^{-i\varepsilon \mathcal{S}_n^{\varepsilon}} \in \mathcal{P}(\mathcal{D}_f, \mathcal{H}_f) \cdot \mathcal{P}(\mathcal{H}_f, \mathcal{D}_f) \cdot \mathcal{B}_1^{\tau} \cdot \mathcal{P}(\mathcal{H}_f) \subset \mathcal{P}(\mathcal{H}_f) \cap \mathcal{B}_1^{\tau}.$$

In view of the cyclicity of the trace per unit volume, Corollary 3.3(i) and Corollary 3.3(iii), we have that³

$$\tau \left([H_0, X] \Pi_n^{\varepsilon} \right) = \tau \left(\Pi_n^{\varepsilon} [H^{\varepsilon}, X] \Pi_n^{\varepsilon} \right) = \tau \left([\Pi_n^{\varepsilon} H^{\varepsilon} \Pi_n^{\varepsilon}, \Pi_n^{\varepsilon} X \Pi_n^{\varepsilon}] \right) + \varepsilon^{n+1} \tau \left(\Pi_n^{\varepsilon} R_n^{\varepsilon} \left(\Pi_n^{\varepsilon} \right)^{\perp} X \Pi_n^{\varepsilon} - \Pi_n^{\varepsilon} X \left(\Pi_n^{\varepsilon} \right)^{\perp} R_n^{\varepsilon} \Pi_n^{\varepsilon} \right) = \tau \left([\Pi_n^{\varepsilon} H^{\varepsilon} \Pi_n^{\varepsilon}, \Pi_n^{\varepsilon} X \Pi_n^{\varepsilon}] \right) + \varepsilon^{n+1} \tau \left(\Pi_n^{\varepsilon} [[\Pi_n^{\varepsilon}, R_n^{\varepsilon}], [X, \Pi_n^{\varepsilon}]] \Pi_n^{\varepsilon} \right) = \tau \left([\Pi_n^{\varepsilon} H_0 \Pi_n^{\varepsilon}, \Pi_n^{\varepsilon} X \Pi_n^{\varepsilon}] \right) - \varepsilon \tau \left([\Pi_n^{\varepsilon} Y \Pi_n^{\varepsilon}, \Pi_n^{\varepsilon} X \Pi_n^{\varepsilon}] \right) + \varepsilon^{n+1} \tau \left(\Pi_n^{\varepsilon} [[\Pi_n^{\varepsilon}, R_n^{\varepsilon}], [X, \Pi_n^{\varepsilon}]] \Pi_n^{\varepsilon} \right)$$

where the term carrying the prefactor ε^{n+1} is uniformly bounded in ε . Observe that in view of Corollary 3.3(ii) and Proposition 2.5(i) we have that

$$\begin{aligned} \Pi_n^{\varepsilon} H_0 \Pi_n^{\varepsilon} &= \Pi_n^{\varepsilon} H_0 \cdot (\mathrm{e}^{\mathrm{i}\varepsilon \mathcal{S}_n^{\varepsilon}} - \mathbb{1}) \Pi_0 \mathrm{e}^{-\mathrm{i}\varepsilon \mathcal{S}_n^{\varepsilon}} + \Pi_n^{\varepsilon} H_0 \cdot \Pi_0 \mathrm{e}^{-\mathrm{i}\varepsilon \mathcal{S}_n^{\varepsilon}} \\ &\in \mathcal{P}(\mathcal{H}_{\mathrm{f}}, \mathcal{D}_{\mathrm{f}}) \cdot \mathcal{P}(\mathcal{D}_{\mathrm{f}}, \mathcal{H}_{\mathrm{f}}) \subset \mathcal{P}(\mathcal{H}_{\mathrm{f}}), \end{aligned}$$

thus Proposition 4.2 implies that the first summand on the right-hand side of (4.1) vanishes. On the other hand, by Corollary 3.3(ii) the unitary $e^{i\epsilon S_n^{\epsilon}}$ is in $\mathcal{P}(\mathcal{H}_f)$, therefore Proposition 4.4 and Remark 4.3 imply that the second summand in (4.1) can be

³ We are allowed to perform all the following algebraic manipulations since the range of $\mathcal{U}_{BFZ\chi_{C_1}}$ is contained in $C_{\rho}^{\infty}(\mathbb{R}^d, \mathcal{H}_f)$ (see Definitions 2.2 and A.1).

rewritten as

$$-\varepsilon \tau ([\Pi_n^{\varepsilon} Y \Pi_n^{\varepsilon}, \Pi_n^{\varepsilon} X \Pi_n^{\varepsilon}]) = \varepsilon \tau ([\Pi_0 X \Pi_0, \Pi_0 Y \Pi_0])$$

= $\varepsilon \tau (\Pi_0 [[\Pi_0, X], [\Pi_0, Y]] \Pi_0).$

This concludes the proof.

Remark 4.5 It is worth pointing out that in the context of spin transport at zero temperature, which is relevant for the quantum Hall spin effect, one can use a similar argument to prove the vanishing of the spin torque in the NEASS up to $\mathcal{O}(\varepsilon^{\infty})$ [31]. Specifically, denoting by S_z the operator representing the z-component of the spin, defined as

$$S_z := \mathbb{1}_{L^2(\mathcal{X})} \otimes s_z$$
, where $s_z = \sigma_z/2$ is half of the third Pauli matrix,

[31, Theorem III.4] shows that under the same hypotheses of Theorem 4.1 one has that for every $n \in \mathbb{N}$

$$\tau\left(\mathrm{i}[H_0, S_z] \Pi_n^{\varepsilon}\right) = \mathcal{O}(\varepsilon^{n+1}).$$

In other words, the *spin torque operator* $i[H_0, S_z]$ has an expectation in the NEASS which vanishes at any order in ε . This result validates the claim in [42] that "one is often interested in a particular component of the spin, and the corresponding torque component can vanish in the bulk on average [...] This is certainly true for the many models used for the study of the spin-Hall effect".

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Appendix A. Trace per unit volume

Here we recall the definition and the main properties of the trace-per-unit-volume functional (for further details, see [35, Sect. 2] and references therein). For any $L \in 2\mathbb{N} + 1$, we define

$$\mathcal{C}_L := \left\{ x \in \mathcal{X} : x = \sum_{j=1}^d \alpha_j \, a_j \text{ with } |\alpha_j| \le L/2 \, \forall \, j \in \{1, \dots, d\} \right\}$$
(A.1)

and $\chi_L := \chi_{\mathcal{C}_L}$, denoting the orthogonal projection on \mathcal{H} which multiplies by the characteristic function of \mathcal{C}_L . In particular, the set \mathcal{C}_1 is called a *fundamental cell*. We say that an operator A acting in \mathcal{H} is *trace class on compact sets* if and only if $\chi_K A \chi_K$ is trace class for all compact sets $K \subset \mathcal{X}^4$.

Definition A.1 (Trace per unit volume). Let A be an operator acting in \mathcal{H} such that A is trace class on compact sets. The *trace per unit volume* of A is defined as

$$\tau(A) := \lim_{\substack{L \to \infty \\ L \in 2\mathbb{N}+1}} \frac{1}{|\mathcal{C}_L|} \operatorname{Tr}(\chi_L A \chi_L),$$
(A.2)

whenever the limit exists.

The most relevant properties of the trace per unit volume are presented in the following results, whose proofs can be found in [35, Sect. 2]. We detail an argument only for Proposition A.3(iv), which is not present in the above reference. We introduce the vector spaces

$$\mathcal{B}_{\infty}^{\tau} := \{ \text{bounded } periodic \text{ operators on } \mathcal{H} \}, \\ \mathcal{B}_{1}^{\tau} := \{ A \in \mathcal{B}_{\infty}^{\tau} \text{ such that } \|A\|_{1,\tau} := \tau(|A|) < \infty \}.$$

We recall that \mathcal{B}_1^{τ} is invariant by left and right multiplication by elements of $\mathcal{B}_{\infty}^{\tau} \supset \mathcal{P}(\mathcal{H}_f)$. Similarly to the standard trace, the trace per unit volume is (conditionally) *cyclic*.

Lemma A.2 (Cyclicity of the trace per unit volume). If $A \in \mathcal{B}_1^{\tau}$ and $B \in \mathcal{B}_{\infty}^{\tau}$, then $\tau(AB) = \tau(BA)$.

The next result collects all the essential properties of the trace per unit volume.

Proposition A.3 (*i*) Let $A \in \mathcal{B}_1^{\tau}$. Then

$$\operatorname{Tr}(|\chi_L A \chi_L|) < \infty \quad \forall L \in 2\mathbb{N} + 1.$$

In particular, we have that A is trace class on compact sets.

⁴ Notice that in the discrete case this condition is automatically satisfied for any operator A because the range of χ_K is finite-dimensional.

(ii) Let A be periodic and trace class on compact sets. Then $\tau(A)$ is well-defined and

$$\tau(A) = \frac{1}{|\mathcal{C}_1|} \operatorname{Tr}(\chi_1 A \chi_1).$$

(iii) Let A be a periodic and bounded operator acting on H. Denoting by

$$\mathcal{U}_{\mathrm{BFZ}} A \, \mathcal{U}_{\mathrm{BFZ}}^{-1} = \int_{\mathbb{R}^d}^{\oplus} \mathrm{d}k \, A(k)$$

its Bloch–Floquet–Zak decomposition, assume that A(k) is trace class and that $\operatorname{Tr}_{\mathcal{H}_{f}}(|A(k)|) < C$ for all $k \in \mathbb{B}^{d}$. Then

$$\operatorname{Tr}(\chi_1 A \chi_1) = \frac{1}{|\mathbb{B}^d|} \int_{\mathbb{B}^d} \mathrm{d}k \ \operatorname{Tr}_{\mathcal{H}_{\mathrm{f}}}(A(k)).$$

(iv) Let $A \in \mathcal{P}(\mathcal{H}_f) \cap \mathcal{B}_1^{\tau}$. Then $\tau([A, X_i])$ is well-defined and $\tau([A, X_i]) = 0$ for every $1 \le i \le d$.

Proof(*iv*) By Lemma 2.3, we have that $[A, X_i] \in \mathcal{P}(\mathcal{H}_f)$. Observe that the operator

$$\chi_L[A, X_i]\chi_L = \chi_L A \chi_L X_i \chi_L - \chi_L X_i \chi_L A \chi_L$$
 is trace class on compact sets,

by applying Proposition A.3(i) and noticing that $\chi_L X_i \chi_L$ is bounded. Thus, Proposition A.3(ii) implies that

$$|\mathcal{C}_1| \cdot \tau([A, X_i]) = \operatorname{Tr}(\chi_1[A, X_i]\chi_1) = \operatorname{Tr}(\chi_1A\chi_1X_i\chi_1 - \chi_1X_i\chi_1A\chi_1),$$

where both summands inside the trace are trace class because $\chi_1 A \chi_1$ is trace class. The cyclicity of the standard trace concludes the proof.

Appendix B. Inverse Liouvillian

Here we recall the expression of the inverse Liouvillian $\mathscr{L}_{H_0}^{-1}$, associated with the unperturbed Hamiltonian H_0 , and its relevant properties.

We look for the solution *B* to the equation $\mathscr{L}_{H_0}(B) = -i[H_0, B] = A$, where $A = A^{OD} \in \mathcal{P}(\mathcal{H}_f)$ is off-diagonal with respect to the decomposition $\mathcal{H} = \operatorname{Ran} \Pi_0 \oplus (\operatorname{Ran} \Pi_0)^{\perp}$. We state in the following Proposition, whose proof can be found in [35, Subsection 6.2], the solution to this problem, which traces back at least to [3, Equation (2.11)] (see also [25, Equation (A10)]).

Proposition B.1 Under Assumption 2.4, let $A \in \mathcal{P}(\mathcal{H}_f)$ be such that $A = A^{OD}$ with respect to Π_0 . Then, the unique off-diagonal solution in $\mathcal{P}(\mathcal{H}_f, \mathcal{D}_f)$ to the equation

$$\mathscr{L}_{H_0}(B) = -\mathrm{i}[H_0, B] = A \quad on \quad \mathcal{U}_{\mathrm{BFZ}}^{-1} L^2_o(\mathbb{R}^d, \mathcal{D}_{\mathrm{f}}),$$

is given by

$$B = \mathscr{L}_{H_0}^{-1}(A) := \frac{1}{2\pi} \oint_C dz \, (H_0 - z\mathbb{1})^{-1} \, [\Pi_0, A] \, (H_0 - z\mathbb{1})^{-1}. \tag{B.1}$$

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