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Spin Conductance and Spin Conductivity in Topological Insulators: Analysis of Kubo-Like Terms

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Abstract. We investigate spin transport in 2-dimensional insulators, with the long-term goal of establishing whether any of the transport coefficients corresponds to the Fu–Kane–Mele index which characterizes $2d$ time-reversal-symmetric topological insulators. Inspired by the Kubo theory of charge transport, and by using a proper definition of the spin current operator (Shi et al. in Phys Rev Lett 96:076604, 2006), we define the Kubo-like spin conductance $G_K^{s_z}$ and spin conductivity $\sigma_K^{s_z}$. We prove that for any gapped, periodic, near-sighted discrete Hamiltonian, the above quantities are mathematically well defined and the equality $G_K^{s_z} = \sigma_K^{s_z}$ holds true. Moreover, we argue that the physically relevant condition to obtain the equality above is the vanishing of the mesoscopic average of the spin-torque response, which holds true under our hypotheses on the Hamiltonian operator. A central role in the proof is played by the trace per unit volume and by two generalizations of the trace, the *principal value trace* and its directional version.

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1. Introduction

The last few decades witnessed an increasing interest, among solid state physicists, for physical phenomena having a topological origin. This interest traces back to the milestone paper by Thouless, Kohmoto, Nightingale and den Nijs on the quantum Hall effect (QHE) [49], includes the pioneering work of Haldane on Chern insulators [23] and the seminal papers by Fu, Kane and Mele concerning the quantum spin Hall effect (QSHE) [18,19,25,26] up to the most recent developments in the flourishing field of topological insulators [2,25,30,37,44].

As it is well known, in the QHE a topological invariant (Chern number) is related to an observable quantity, the transverse charge conductance or Hall conductance. By analogy, in the context of the QSHE for 2-dimensional time-reversal-symmetric insulators, one would like to connect—if possible—the relevant topological invariant (Fu–Kane–Mele index) to a macroscopically observable quantity. The natural candidates are spin conductance and spin conductivity, whose proper definition has been debated, and whose equivalence has not been yet established.

The first crucial point is to characterize the operator corresponding to the *spin current density*. In the last few years, an intense debate about the correct expression of the latter took place, but a general consensus was not reached [1,10,37,44,46,48,51]. Among the candidates, one may include[1]:

(i) the naive guess

$$\mathbf{J}_{\text{naive}} = \mathrm{i}[H, \mathbf{X}]\, S_z,$$

where H is the Hamiltonian operator of the system, $\mathbf{X} = (X_1, X_2)$ is the position operator, and S_z represents the z-component of the spin;

(ii) its symmetrized version, namely

$$\mathbf{J}_{\text{sym}} = \tfrac{1}{2}\left(\mathbf{J}_{\text{naive}} + \mathbf{J}^*_{\text{naive}}\right) = \tfrac{1}{2}\left(\mathrm{i}[H, \mathbf{X}]\, S_z + \mathrm{i}S_z\, [H, \mathbf{X}]\right),$$

which has the advantage of providing a self-adjoint operator;

(iii) last but not least, the alternative provided by the "proper" spin current

$$\mathbf{J}_{\text{prop}} = \mathrm{i}[H, \mathbf{X}S_z], \tag{1.1}$$

proposed by [46], which is also self-adjoint.

[1]We use Hartree atomic units, so that the reduced Planck constant $\hbar$, the squared electron charge e^2 and the electron mass m_{e} are dimensionless and equal to 1. In particular, the quantum of charge conductivity in the QHE is $\frac{e^2}{h} = \frac{1}{2\pi}$.

Whenever $[H, S_z] = 0$ (spin-commuting case), the three above definitions agree, while they differ in general. Notice that spin conservation is often violated in topological insulators, as it happens e.g. in the paradigmatic model proposed by Kane and Mele [25,26], reviewed in Appendix A. Hence, it is of prominent importance to understand which choice best models the physics, aiming at a closer comparison between the theoretical predictions and the ongoing and challenging experiments on the quantum spin Hall effect [50].

The choice (iii) has the advantage to provide an operator associated to a sourceless continuity equation for the associated density and to Onsager relations [46,51]. On the other hand, whenever H is periodic, $\mathbf{J}_{\mathrm{sym}}$ provides a *periodic* (or covariant, when ergodic randomness is added) operator, while—as early remarked by Schulz-Baldes—the latter property fails to hold for $\mathbf{J}_{\mathrm{prop}}$, which "*leads to technical difficulties, but also questions the physical relevance*" of the operator $\mathbf{J}_{\mathrm{prop}}$ [44].

In this paper, we are inspired by the following simple but new observation: even if $\mathbf{J}_{\mathrm{prop}}$ is not periodic, it satisfies a peculiar commutation relation with the lattice translations $\{T_{\mathbf{p}}\}_{\mathbf{p}\in\mathbb{Z}^d}$ whenever the Hamiltonian operator is periodic. Namely,

$$T_{\mathbf{p}}\,\mathbf{J}_{\mathrm{prop}}\,T_{\mathbf{p}}^{-1} = \mathbf{J}_{\mathrm{prop}} - \mathbf{p}\,\mathrm{i}[H, S_z] \quad \forall \mathbf{p} \in \mathbb{Z}^d. \tag{1.2}$$

Hence, whenever the *spin torque* $\mathrm{i}[H, S_z]$ averages to zero on the mesoscopic scale, e.g. because $\tau\left(\mathrm{i}[H, S_z]\rho(t)\right) = 0$ where $\tau(\,\cdot\,)$ is the trace per unit volume (see Definition 2.6) and $\rho(t)$ is the density matrix describing the state of the system, the operator $\mathbf{J}_{\mathrm{prop}}$ is *"mesoscopically periodic"*, in the sense that its commutator with the lattice translations vanishes on the mesoscopic scale.

A second crucial question is whether the relevant observable quantity related to the Fu–Kane–Mele (FKM) index is the spin conductance, or the spin conductivity, or some other transport coefficient, if any. We recall that the transverse (resp. direct) spin conductance is defined, experimentally, as the ratio between the spin current intensity and the electric potential drop measured in orthogonal (resp. parallel) directions, hence as the ratio of two extensive observable quantities. On the contrary, the transverse (resp. direct) spin conductivity is the ratio between the expectation value per unit volume of spin current and the strength of the electric field measured in orthogonal (resp. parallel) directions, and as such is the ratio of two intensive quantities. In the case of *charge transport* in 2-dimensional systems, the equality of charge conductance and conductivity holds true, as proved in [7] under suitable technical hypotheses, at least within the linear response approximation (LRA) [3,4,21]. In the case of *spin transport*, the situation is instead radically different and, unless $[H, S_z] = 0$, it is not obvious a priori whether the equality between spin conductance and spin conductivity holds true or not.

Our analysis encompasses several steps. As a first step, we reconsider the spin transport starting from the first principles of quantum mechanics. This analysis, performed in two related papers [32,33] by a space- and a time-adiabatic approach, respectively, shows that spin conductivity and conductance, defined by using the operator $\mathbf{J}_{\mathrm{prop}}$ (whose lack of periodicity is harmless on the mesoscopic scale, as remarked above), contain additional terms with respect to what suggested by the analogy with the Kubo theory of charge transport. The physical relevance of the additional terms is at the moment unclear and deserves further investigations by both numerical and analytical methods.

As a second step, in this paper we investigate the *Kubo-like terms*. Explicitly, they are the following:

(a) the *Kubo-like spin conductivity* is defined as

$$\sigma_K^{s_z} := \tau(\Sigma_K^{s_z}) \quad \text{with} \quad \Sigma_K^{s_z} := \mathrm{i}P\left[[P, X_1 S_z], [P, X_2]\right]P \tag{1.3}$$

where P is the Fermi projector up to energy $\mu \in \mathbb{R}$, which is supposed to be in a spectral gap, and $\tau(\,\cdot\,)$ is the trace per unit volume (TUV). The fact that $\tau(\Sigma_K^{s_z})$ is well defined and finite will be part of our results.

(b) the *Kubo-like spin conductance* is defined as

$$G_K^{s_z}(\Lambda_1, \Lambda_2) := 1\text{-pvTr}\big(\mathcal{G}_K^{s_z}(\Lambda_1, \Lambda_2)\big)$$
$$\text{with } \mathcal{G}_K^{s_z}(\Lambda_1, \Lambda_2) := \mathrm{i}P\left[[P, \Lambda_1 S_z], [P, \Lambda_2]\right]P \tag{1.4}$$

where Λ_j is a switch function in direction $j \in \{1, 2\}$, as in Definition 2.3. The fact that the operator $\mathcal{G}_K^{s_z}(\Lambda_1, \Lambda_2)$ is not trace class (see Remark 4.8), forces us to introduce a suitable trace-like linear functional, denoted by 1-pvTr$(\,\cdot\,)$ and baptized *directional principal value trace* in direction $j = 1$ in Definition 2.5, which generalizes the trace.

The new result of our paper is that for any gapped, *periodic*, and near-sighted Hamiltonian (compare Assumption 2.2), one has the equality

$$G_K^{s_z}(\Lambda_1, \Lambda_2) = \sigma_K^{s_z}.$$

In particular, under these assumptions, the spin conductance is independent of the switch functions Λ_1 and Λ_2 involved in its definition. The precise results, which for technical reasons are proved in the setting of discrete Hamiltonian operators, are stated in Theorems 2.8 and 2.9, while the crucial observation mentioned after (1.2) reflects in Eqs. (2.4), (3.2) and (5.20) in the proofs. Notice that our results do not assume the smallness of $[H, S_z]$; hence, they go beyond the regime of spin quasi-conservation considered in previous papers [40, 44].

Moreover, the structure of the proof suggests that, more generally, spin conductance and conductivity are equal under the more general condition that $\tau(\mathcal{T}_{s_z}) = 0$, where the *spin-torque response* operator is defined by

$$\mathcal{T}_{s_z} := \mathrm{i}P\left[[P, S_z], [P, X_2]\right]P. \tag{1.5}$$

Physically, $\tau(\mathcal{T}_{s_z})$ represents—within LRA—the response of the system, in terms of spin torque $\mathrm{i}[H, S_z]$, to a uniform electric field in direction 2. Indeed, the term $[P, X_2]$ originates from the perturbation by a linear potential, i.e. a uniform electric field, whereas $[P, S_z]$ stands for the spin-torque response, namely the response in the expectation value of $\mathrm{i}[H, S_z]$, to this perturbation.

To prove our results, we need to set up a suitable mathematical machinery, involving some trace-like linear functionals, as the *principal value trace* (Definition 2.4) and the *j-directional principal value trace* (Definition 2.5). We also prove some relevant properties of the trace per unit volume (Definition 2.6).
As it is well known, in an infinite-dimensional Hilbert space one has in general $\mathrm{Tr}([A,B]) \neq 0$, since the cyclicity of the trace holds true only under special conditions, e.g. if AB and BA are trace class and both A and B are bounded operators [47, Corollary 3.8]. Similar subtleties appear when considering the trace-like functionals mentioned above. It is noteworthy that many physically relevant quantities appear as the trace or TUV of exact commutators. For example, as noticed in [7] the Kubo charge conductance σ_K^e for a quantum Hall system can be rewritten as

$$\sigma_K^e = \mathrm{i}\,\tau\big([PX_1P, PX_2P]\big)$$

where P is the spectral projector up to the Fermi energy. Hence, the mentioned mathematical subtleties are not an abstract academic issue, but are deeply intertwined with the physics of quantum transport. For this reason, we devote two sections to the analysis of the properties of the mentioned trace-like functionals (Sects. 3, 4), also considering that part of this machinery might be of independent interest. In this analysis, we greatly benefited by the previous work on charge transport in quantum Hall systems, including in particular [3,6–9,14,15]. The mathematical setting and the main results are discussed in Sect. 2, while Sect. 5 is devoted to the proofs.

Our work provides a mathematical consistent expression for the Kubo-like terms of spin conductivity and conductance, and some sufficient conditions which imply their equality. Moreover, our work puts on solid mathematical grounds the proposal to use $\mathbf{J}_{\mathrm{prop}}$ as the self-adjoint operator corresponding to spin current density, circumventing the criticism related to its failure to be periodic. These results pave the way to further developments in the mathematical theory of time-reversal-symmetric topological insulators, a very active field of research in Solid State Physics and, more recently, in Mathematical Physics [5,11–13,16,17,20,22,27,34,35,40,41,44,45].

2. Setting and Main Results

We consider independent electrons moving in a discrete set $\mathcal{C} \subset \mathbb{R}^2$, which is supposed to be a *periodic crystal*, i.e. it is equipped with a free action of a Bravais lattice $\Gamma \simeq \mathbb{Z}^2$. In view of the latter action, after a choice of a periodicity cell, one decomposes $\mathcal{C} \simeq \mathbb{Z}^2 \times \{\nu_1, \dots, \nu_N\}$, where the second factor corresponds to the "points inside the chosen periodicity cell" (see Appendix A for the specific case of the honeycomb structure and the Kane–Mele model).

Taking spin into account, the Hilbert space of the system is $\mathcal{H}_{\mathrm{phys}} = \ell^2(\mathcal{C}) \otimes \mathbb{C}^2$ which, in view of the above procedure, is identified with

$$\mathcal{H}_{\mathrm{disc}} = \ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^N \otimes \mathbb{C}^2. \tag{2.1}$$

Any bounded operator A acting on $\mathcal{H}_{\text{disc}}$ is characterized by a collection of matrices $\{A_{\mathbf{n},\mathbf{m}}\}_{\mathbf{n},\mathbf{m}\in\mathbb{Z}^2} \subset \operatorname{End}(\mathbb{C}^N \otimes \mathbb{C}^2)$. We denote by $|A_{\mathbf{m},\mathbf{n}}|$ the corresponding matrix norm, while the operator norm on the full Hilbert space $\mathcal{H}_{\text{disc}}$ is denoted by $\|A\|$.

Definition 2.1. A bounded operator A acting on $\mathcal{H}_{\text{disc}}$ is called *near-sighted*[2] if and only if there exist constants $C, \zeta > 0$ such that

$$|A_{\mathbf{m},\mathbf{n}}| \leq C\mathrm{e}^{-\frac{1}{\zeta}\|\mathbf{m}-\mathbf{n}\|_1} \quad \forall \mathbf{m}, \mathbf{n} \in \mathbb{Z}^2,$$

where $\|\mathbf{n}\|_1 := \sum_{j=1}^{2} |n_j|$. The constant ζ is called the *range* of A.

Assumption 2.2. The Hamiltonian operator H is a bounded self-adjoint operator acting on $\mathcal{H}_{\text{disc}}$. Further, we assume that the operator H

(H_1) is near-sighted with range ζ_H;
(H_2) is periodic, namely $H_{\mathbf{m},\mathbf{n}} = H_{\mathbf{m}-\mathbf{p},\mathbf{n}-\mathbf{p}}$ for all $\mathbf{m}, \mathbf{n}, \mathbf{p} \in \mathbb{Z}^2$;
(H_3) admits a spectral gap, namely there exist non-empty sets $I_1, I_2 \subseteq \mathbb{R}$ and $a, b \in \mathbb{R}$, such that

$$\operatorname{Spectrum}(H) = I_1 \cup I_2 \text{ and } \sup I_1 < a < b < \inf I_2.$$

The interval $\Delta = (\inf a, \sup b)$ is called the **spectral gap**.

For $\mu \in \Delta$, we denote the Fermi projection by

$$P := \chi_{(-\infty,\mu)}(H), \tag{2.2}$$

where χ_Ω is the characteristic function of the set Ω. In Appendix A, we show that the Hamiltonian H_{KM} of the Kane–Mele model, which is often considered the paradigmatic model of time-reversal-symmetric topological insulators, enjoys all the above assumptions, whenever the values of the parameters guarantee the existence of a spectral gap. Moreover, one easily sees that $[H_{\text{KM}}, S_z] \neq 0$.

The aim of this paper is to analyze the Kubo-like terms in the spin conductivity and spin conductance, defined as in (1.3) and (1.4), respectively. In our context, the position operator $\mathbf{X} = (X_1, X_2)$ acts in $\mathcal{H}_{\text{disc}}$ as

$$(X_j\varphi)_{\mathbf{n}} := n_j\varphi_{\mathbf{n}}, \quad j \in \{1, 2\}, \quad \forall \varphi \in \mathcal{D}(X_j).$$

The spin operator S_z acts on $\mathcal{H}_{\text{disc}}$ as $\mathbb{1} \otimes \mathbb{1} \otimes \frac{1}{2}s_z$, where s_z is the third Pauli matrix. In order to keep a light notation, in the following we identify any operator A which acts only in one sector of $\mathcal{H}_{\text{disc}}$, with the one acting in $\mathcal{H}_{\text{disc}}$ with extra identity factors, and we keep the same notation A (e.g. $X_1 \equiv X_1 \otimes \mathbb{1}_{\mathbb{C}^N} \otimes \mathbb{1}_{\mathbb{C}^2}$, and so on).

The operator $\mathcal{G}_K^{s_z}$ involves the notion of switch function, which we now define.

[2]The term near-sighted was proposed by the Nobel Laureate Walter Kohn [30,39], in a slightly different context. For electrons in crystals, "it describes the fact that [...] local electronic properties [...] depend significantly on the effective external potential only at nearby points." The term *short range operator* is often equivalently used in the literature, as well as *local operator*. The latter use, however, overlaps with the standard meaning of the word "local" in the theory of operators, so we avoid it.

Definition 2.3. Fix $j \in \{1,2\}$. A *switch function in the* jth-*direction* is a function $\Lambda_j\colon \mathbb{Z}^2 \to [0,1]$ that depends only on the variable n_j and satisfies

$$\Lambda_j(n_j) = \begin{cases} 0 & \text{if } n_j < n_- \\ 1 & \text{if } n_j \geq n_+ \end{cases}$$

for arbitrary $n_- < n_+$.

In the following, we will identify a function defined on $\mathbb{Z}^2$ with the corresponding multiplication operator on $\ell^2(\mathbb{Z}^2)$.

As anticipated in the introduction, many subtleties of the quantum theory of transport arise since some relevant operators appearing in the theory are not trace class. The operators $\Sigma_K^{s_z}$ and $\mathcal{G}_K^{s_z}$, defined in (1.3) and (1.4), are not exceptional. To overcome this problem, one needs to define suitable trace-like linear functionals corresponding to the relevant physical quantities. The transverse spin conductivity is defined through the well-known trace per unit volume. However, for the conductance the situation is quite different and we have to introduce the notions of *principal value trace* and its *directional* version.

We make use of the norm

$$\|\mathbf{n}\|_\infty := \max_{j\in\{1,2\}} |n_j| \quad \forall \mathbf{n} \in \mathbb{Z}^2,$$

which conveniently respects the square structure of $\mathbb{Z}^2$. For any $L \in 2\mathbb{N}+1$ and $\mathbf{n}_0 \in \mathbb{Z}^2$, we set

$$\mathcal{Q}_L(\mathbf{n}_0) := \left\{\mathbf{n} \in \mathbb{Z}^2\colon \|\mathbf{n} - \mathbf{n}_0\|_\infty \leq L/2\right\}$$

to denote the square of side L centered at $\mathbf{n}_0$. Following [9], we restrict to odd integers ($L \in 2\mathbb{N}+1$) in order to use the convenient decomposition[3]

$$\mathcal{Q}_L(\mathbf{n}_0) = \bigsqcup_{\mathbf{n}\in\mathcal{Q}_L(\mathbf{n}_0)} \mathcal{Q}_1(\mathbf{n}). \tag{2.3}$$

For the sake of better readability, we write $\mathcal{Q}_L$ for $\mathcal{Q}_L(\mathbf{0})$.
We denote by $\chi_L := \chi_{\mathcal{Q}_L}$, for $L \in 2\mathbb{N}+1$, the characteristic function of the square $\mathcal{Q}_L$, and by $\chi_{j,L}$, for $j \in \{1,2\}$ and $L \in 2\mathbb{N}+1$, the characteristic function of the stripe $\left\{\mathbf{m} \in \mathbb{Z}^2\colon |m_j| \leq L/2\right\}$.

Definition 2.4 (*Principal value trace*). Let A be an operator acting in $\mathcal{H}_{\mathrm{disc}}$ such that[4] $\chi_L A \chi_L$ is trace class for every $L \in 2\mathbb{N}+1$. The principal value trace of A, is defined, whenever the limit exists, as

$$\mathrm{pvTr}(A) := \lim_{\substack{L\to\infty \\ L\in 2\mathbb{N}+1}} \mathrm{Tr}(\chi_L A \chi_L).$$

[3] The symbol $\bigsqcup$ corresponds to the disjoint union.
[4] The condition that "$\chi_L A \chi_L$ is trace class for every $L \in 2\mathbb{N}+1$" is automatically satisfied in every discrete model, as those considered in this paper, since the range of χ_L is finite-dimensional. We decided to state this redundant condition anyhow, since we prefer to consider the same definition for discrete and continuum models (Schrödinger operators), as we plan to extend the proof to the latter models in the future.

Notice that the principal value trace was already used in the context of quantum Hall effect [7, Definition 6.6], but not its directional version that is used below. As we deal with a two-dimensional system, we can also define the notion of directional principal value trace depending on the jth-direction, where $j \in \{1, 2\}$ indicates the direction around which one localizes.

Definition 2.5 (*Directional principal value trace*). Fix an index $j \in \{1, 2\}$. Let A be an operator acting in $\mathcal{H}_{\mathrm{disc}}$ such that $\chi_{j,L} A \chi_{j,L}$ is trace class for every $L \in 2\mathbb{N} + 1$. The j-directional principal value trace of A, is defined, whenever the limit exists, as

$$j\text{-pvTr}(A) := \lim_{\substack{L \to \infty \\ L \in 2\mathbb{N}+1}} \mathrm{Tr}(\chi_{j,L} A \chi_{j,L}).$$

We will show in Sect. 3 that both the principal value trace and its directional version coincide with the usual trace whenever A is a trace class operator. However, these functionals work also for operators which are not trace class, in analogy with generalized integrals. Finally, we recall the definition of trace per unit volume (see [4,9] and references therein).

Definition 2.6 (*Trace per unit volume*). Let A be an operator acting in $\mathcal{H}_{\mathrm{disc}}$ such that (see footnote 4) $\chi_L A \chi_L$ is trace class for every $L \in 2\mathbb{N}+1$. The trace per unit volume of A, is defined, whenever the limit exists, as

$$\tau(A) := \lim_{\substack{L \to \infty \\ L \in 2\mathbb{N}+1}} \frac{1}{L^2} \mathrm{Tr}(\chi_L A \chi_L).$$

The fundamental properties of these three trace-like linear functionals are discussed in Sect. 3.

We now state an auxiliary lemma and then discuss the main results of the paper.

Lemma 2.7. *Let H be as in Assumption 2.2 and P be the corresponding Fermi projection, as in (2.2). Then, the spin-torque response operator*

$$\mathcal{T}_{s_z} = \mathrm{i} P \left[[P, S_z], [P, X_2] \right] P$$

is periodic and bounded. Moreover, $\mathcal{T}_{s_z}$ has finite trace per unit volume and it holds

$$\tau(\mathcal{T}_{s_z}) = \mathrm{Tr}(\chi_1 \mathcal{T}_{s_z} \chi_1).$$

*$\tau(\mathcal{T}_{s_z})$ is called the **mesoscopic average of spin-torque response**.*

Theorem 2.8 (Vanishing of spin-torque response). *Let H be as in Assumption 2.2 and P be the corresponding Fermi projection, as in (2.2). Then,*

$$\tau(\mathcal{T}_{s_z}) = 0.$$

The physical interpretation of this result is that a uniform electric field does not induce any particular spin-torque excess in the sample, at least within LRA, when averaging on a mesoscopic scale (as done by the trace per unit volume). The proof of it relies on the conditional cyclicity of TUV which, while false in general, holds true for a specific class of operators, as proved in Proposition 3.5.

Theorem 2.9. *Let H be as in Assumption 2.2 and P the corresponding Fermi projection. Then:*

(1) *Let Λ_2 be a fixed switch function in the* 2nd-*direction. Assume that $G_K^{s_z}(\Lambda_1, \Lambda_2)$, defined by (1.4), is finite for at least a switch function Λ_1. Then, $G_K^{s_z}(\Lambda_1', \Lambda_2)$ is finite for any switch function Λ_1', and it is independent of the choice of Λ_1'.*

(2) *The operator $\Sigma_K^{s_z}$, defined in (1.3), satisfies*

$$(\Sigma_K^{s_z})_{\mathbf{m},\mathbf{n}} = (\Sigma_K^{s_z})_{\mathbf{m}-\mathbf{p},\mathbf{n}-\mathbf{p}} - p_1 (\mathcal{T}_{s_z})_{\mathbf{m}-\mathbf{p},\mathbf{n}-\mathbf{p}} \quad \text{for all } \mathbf{m},\mathbf{n},\mathbf{p} \in \mathbb{Z}^2, \tag{2.4}$$

where $\mathcal{T}_{s_z}$ is the spin-torque response defined in (1.5). Moreover, the Kubo-like term in the transverse spin conductivity, defined as $\sigma_K^{s_z} := \tau(\Sigma_K^{s_z})$, is well defined and satisfies

$$\sigma_K^{s_z} = \mathrm{Tr}(\chi_1 \Sigma_K^{s_z} \chi_1).$$

(3) *Finally, the equality*

$$\sigma_K^{s_z} = G_K^{s_z}(\Lambda_1, \Lambda_2) \tag{2.5}$$

holds true. In particular, $G_K^{s_z}$ is finite and independent of the choice of the switch functions Λ_1, Λ_2 in both directions.

Remark 2.10. Before proving the above statements, a few comments are in order.

(i) Notice that the operator $\Sigma_K^{s_z}$ is, in general, not periodic; hence, the fact that its trace per unit volume is well defined and finite, as proved in Theorem 2.9 (2), is not trivial.

(ii) The simplicity of formula (2.5) might obscure the physics of the problem. Indeed, during the proof, one shows that it holds true [see Eq. (5.20)]

$$G_K^{s_z}(\Lambda_1, \Lambda_2) = \sigma_K^{s_z} + \frac{1}{2} \lim_{\substack{L\to\infty \\ L\in 2\mathbb{N}+1}} \sum_{\substack{m_1\in\mathbb{Z} \\ |m_1|\le L/2}} \tau(\mathcal{T}_{s_z}). \tag{2.6}$$

The second summand is a series of constant terms, which is either zero if $\tau(\mathcal{T}_{s_z}) = 0$, or divergent otherwise. As stated in Theorem 2.8, for a gapped *periodic* near-sighted Hamiltonian, one has always $\tau(\mathcal{T}_{s_z}) = 0$. On the other hand, we suspect that Eq. (2.6) is valid in a broader context.

(iii) Whenever

$$[H, S_z] = 0, \tag{2.7}$$

the spin-torque response operator vanishes, see (1.5). In this particular case, it is straightforward to prove that $G_K^{s_z}(\Lambda_1, \Lambda_2) = \sigma_K^{s_z}$, since the proof boils down to the analogous proof for charge transport (see [7] for the continuum case, and [31] for a recent overview of the literature).

In view of (2.7), P admits the decomposition induced by the S_z-eigenspaces, namely

$$P = P_\uparrow \oplus P_\downarrow.$$

In the above, $P_\uparrow$ and $P_\downarrow$ are both projections on $\ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^N$. In this specific case, if H enjoys Assumption 2.2 and is time-reversal symmetric, namely $\Theta H \Theta^{-1} = H$ for $\Theta = \mathrm{e}^{\mathrm{i}\pi s_y/2} K$, where s_y is the second Pauli matrix and K is the natural complex conjugation on $\mathcal{H}_{\mathrm{disc}}$, one has that

$$\sigma_K^{s_z} = \mathrm{i}\tau\big(P\big[[P, X_1],\, [P, X_2]\big] S_z P\big) \\ = \frac{1}{2}\big(C_1(P_\uparrow) - C_1(P_\downarrow)\big) = C_1(P_\uparrow), \tag{2.8}$$

with

$$C_1(P_s) := \frac{\mathrm{i}}{2\pi} \int_{\mathbb{B}} \mathrm{d}k \ \mathrm{tr}\left(P_s(k)[\partial_1 P_s(k), \partial_2 P_s(k)]\right) \quad \text{for } s \in \{\uparrow, \downarrow\},$$

where $P_s(k)$ refers to the fiber operator at fixed crystal momentum, with respect to the modified Bloch–Floquet transform (see e.g. [34,38]). Hence, in the spin-commuting case our result agrees with previous contributions [40,44,45], yielding that the Kubo-like spin conductivity, given by (2.8), agrees with the Spin-Chern number. Moreover, formula (2.8) agrees with the Fu–Kane–Mele index modulo 2 [18,25,45].

3. Machinery: (Directional) Principal Value Trace and Trace Per Unit Volume

In this section, we state and prove some fundamental properties of the trace-like functionals introduced before. First, we recall some facts about the trace and its conditional cyclicity.

Proposition 3.1 (Conditional cyclicity of the trace [47, Corollary 3.8]). *Let $\mathcal{H}$ be a separable Hilbert space. If $A, B \in \mathcal{B}(\mathcal{H})$ have the property that both AB and BA are in the trace class ideal $\mathcal{B}_1(\mathcal{H})$ then*

$$\mathrm{Tr}(AB) = \mathrm{Tr}(BA).$$

Hereafter, the trace on the Hilbert space $\mathcal{H}_{\mathrm{disc}}$ will be denoted by $\mathrm{Tr}\, A$, for any trace class operator A, while the (matrix) trace on $\mathbb{C}^N \otimes \mathbb{C}^2 \simeq \mathbb{C}^{2N}$ by $\mathrm{tr}(\,\cdot\,)$.

If an operator A is trace class, its trace can be computed through the diagonal elements in the position basis of $\ell^2(\mathbb{Z}^2)$, namely $\mathrm{Tr}(A) = \sum_{\mathbf{n}\in\mathbb{Z}^2} \mathrm{tr}(A_{\mathbf{n},\mathbf{n}})$, the latter series being absolutely convergent. We say that $\mathrm{Tr}(A)$ is computed "through the diagonal kernel". The construction of the trace is somehow analogous to the construction of the Lebesgue integral [42, Section VI.6]. As well known, whenever a function is Lebesgue integrable, then its principal value integral exists and it is equal to the Lebesgue integral. Similarly, the (directional) principal value trace is a natural extension of the trace.

Lemma 3.2. *If $A \in \mathcal{B}_1(\mathcal{H}_{\mathrm{disc}})$ then* $\mathrm{pvTr}(A)$ *and* j-$\mathrm{pvTr}(A)$ *are well defined and*

$$\mathrm{pvTr}(A) = \mathrm{Tr}(A) = j\text{-}\mathrm{pvTr}(A).$$

Proof. By the diagonal kernel computation

$$\begin{aligned}\operatorname{Tr}(A) &= \sum_{\mathbf{n}\in\mathbb{Z}^2} \operatorname{tr}(A_{\mathbf{n},\mathbf{n}}) = \lim_{\substack{L\to\infty\\ L\in 2\mathbb{N}+1}} \sum_{\substack{\mathbf{n}\in\mathbb{Z}^2\\ \|\mathbf{n}\|_\infty\le L/2}} \operatorname{tr}(A_{\mathbf{n},\mathbf{n}})\\ &= \lim_{\substack{L\to\infty\\ L\in 2\mathbb{N}+1}} \operatorname{Tr}(\chi_L A \chi_L) = \operatorname{pvTr}(A). \end{aligned} \tag{3.1}$$

The absolute convergence of the series also allows us to compute it as a limit of partial sum in one direction only, leading to j-$\operatorname{pvTr}(A)$ by Fubini's Theorem. □

In the following, we give two sufficient conditions for the existence of the trace per unit volume of an operator: the first one (periodicity) is well known [4,9], while the second one is, to our knowledge, new.

Proposition 3.3 (Existence of TUV, condition I). *Let A be a periodic operator acting in $\mathcal{H}_{\mathrm{disc}}$ such that (see footnote 4) $\chi_L A \chi_L$ is trace class for every $L \in 2\mathbb{N}+1$. Then, $\tau(A)$ is well defined and*

$$\tau(A) = \operatorname{Tr}(\chi_1 A \chi_1).$$

Proof. The operator $\chi_L A \chi_L$ is trace class for every $L \in 2\mathbb{N}+1$, and its trace can be computed through the diagonal kernel. In view of periodicity, one has $A_{\mathbf{n},\mathbf{n}} = A_{\mathbf{0},\mathbf{0}}$ for all $\mathbf{n} \in \mathbb{Z}^2$. Therefore, by using decomposition (2.3), one obtains

$$\operatorname{Tr}(\chi_L A \chi_L) = \sum_{\substack{\mathbf{n}\in\mathbb{Z}^2\\ \|\mathbf{n}\|_\infty\le L/2}} \operatorname{tr}(A_{\mathbf{n},\mathbf{n}}) = L^2 \operatorname{tr}(A_{\mathbf{0},\mathbf{0}}).$$

Hence $\lim_{L\to\infty} \frac{1}{L^2} \operatorname{Tr}(\chi_L A \chi_L) = \operatorname{tr}(A_{\mathbf{0},\mathbf{0}}) = \operatorname{Tr}(\chi_1 A \chi_1)$. □

Proposition 3.4 (Existence of TUV, condition II). *Let A, B be operators acting in $\mathcal{H}_{\mathrm{disc}}$ such that (see footnote 4) $\chi_L A \chi_L$ and $\chi_L B \chi_L$ are trace class for every $L \in 2\mathbb{N}+1$ and satisfy the following equation*

$$A_{\mathbf{m},\mathbf{n}} = A_{\mathbf{m}-\mathbf{p},\mathbf{n}-\mathbf{p}} + g(\mathbf{p})\, B_{\mathbf{m}-\mathbf{p},\mathbf{n}-\mathbf{p}} \quad \text{for all } \mathbf{m},\mathbf{n},\mathbf{p} \in \mathbb{Z}^2, \tag{3.2}$$

where either[5] $\operatorname{tr}(B_{\mathbf{0},\mathbf{0}}) = 0$ *or* $g\colon \mathbb{Z}^2 \to \mathbb{R}$ *is an odd function in at least one variable.*[6] *Then, $\tau(A)$ is well defined and*

$$\tau(A) = \operatorname{Tr}(\chi_1 A \chi_1).$$

Proof. The operator $\chi_L A \chi_L$ is trace class, and we compute its trace through the diagonal kernel. In view of Eq. (3.2), one has $A_{\mathbf{n},\mathbf{n}} = A_{\mathbf{0},\mathbf{0}} + g(\mathbf{n})\, B_{\mathbf{0},\mathbf{0}}$. Therefore, using decomposition (2.3), we obtain

[5] Notice that if B is periodic then $\operatorname{tr}(B_{\mathbf{0},\mathbf{0}}) = \tau(B)$ by Proposition 3.3. However, periodicity is not required here.

[6] Namely, setting $(R_1 g)(n_1, n_2) := g(-n_1, n_2)$ and $(R_2 g)(n_1, n_2) := g(n_1, -n_2)$ for all $\mathbf{n} \in \mathbb{Z}^2$, one says that $g\colon \mathbb{Z}^2 \to \mathbb{R}$ is an odd function in at least one variable if and only if there exists an index $j \in \{1, 2\}$ such that $g(\mathbf{n}) = -(R_j g)(\mathbf{n})$ for all $\mathbf{n} \in \mathbb{Z}^2$.

$$\begin{aligned}\mathrm{Tr}(\chi_L A \chi_L) &= \sum_{\substack{\mathbf{n}\in\mathbb{Z}^2\\ \|\mathbf{n}\|_\infty\le L/2}} \mathrm{tr}(A_{\mathbf{n},\mathbf{n}})\\ &= L^2\,\mathrm{tr}(A_{\mathbf{0},\mathbf{0}}) + \mathrm{tr}(B_{\mathbf{0},\mathbf{0}}) \sum_{\substack{\mathbf{n}\in\mathbb{Z}^2\\ \|\mathbf{n}\|_\infty\le L/2}} g(\mathbf{n}). \end{aligned} \tag{3.3}$$

If $\mathrm{tr}(B_{\mathbf{0},\mathbf{0}}) = 0$ the second summand on the right-hand side vanishes. Otherwise, if the function g is odd in at least one variable, there exists an index $j \in \{1, 2\}$ such that $g(\mathbf{n}) = -(R_j g)(\mathbf{n})$, where R_j is the corresponding reflection (see footnote 6). Denoting by k the index different from j, we have

$$\sum_{\substack{\mathbf{n}\in\mathbb{Z}^2\\ \|\mathbf{n}\|_\infty\le L/2}} g(\mathbf{n}) = \sum_{\substack{n_k\in\mathbb{Z}\\ |n_k|\le L/2}} \sum_{\substack{n_j\in\mathbb{Z}\\ |n_j|\le L/2}} g(\mathbf{n}) = 0.$$

As $\mathrm{tr}(B_{\mathbf{0},\mathbf{0}}) = \mathrm{Tr}(\chi_1 B \chi_1)$ is finite by hypothesis, the second summand on the right-hand side of (3.3) vanishes. □

Proposition 3.5 (Conditional cyclicity of TUV). *Let A, B be periodic operators acting in $\mathcal{H}_{\mathrm{disc}}$ such that (see footnote 4) $\chi_L AB \chi_L$ and $\chi_L BA \chi_L$ are trace class for every $L \in 2\mathbb{N}+1$. Then,*

$$\tau(AB) = \tau(BA).$$

Proof. Applying Proposition 3.3 and computing the trace of $\chi_1 AB \chi_1$ through the diagonal kernel, we have $\tau(AB) = \sum_{\mathbf{n}\in\mathbb{Z}^2} \mathrm{tr}\, A_{\mathbf{0},\mathbf{n}} B_{\mathbf{n},\mathbf{0}}$. We conclude the proof by using the periodicity of A and B, the change of variable $\mathbf{n} \mapsto -\mathbf{n}$ and the cyclicity of $\mathrm{tr}(\,\cdot\,)$ on a finite-dimensional Hilbert space. □

4. Localization Properties of Near-Sighted Operators

In this section, we consider the peculiar localization properties of operators which are near-sighted, see Definition 2.1, and their relation with the trace class condition. Preliminarily, we recall some results which are useful to establish the trace class property in the discrete case [14].

Remark 4.1 (**Hölmgren's estimate**). For an operator A acting on $\mathcal{H}_{\mathrm{disc}}$

$$\|A\| \le \max\left(\sup_{\mathbf{m}\in\mathbb{Z}^2} \sum_{\mathbf{n}\in\mathbb{Z}^2} |A_{\mathbf{m},\mathbf{n}}|\,,\ \sup_{\mathbf{n}\in\mathbb{Z}^2} \sum_{\mathbf{m}\in\mathbb{Z}^2} |A_{\mathbf{m},\mathbf{n}}| \right).$$

Definition 4.2. A function $f\colon \mathbb{Z}^2 \to \mathbb{R}$ is called *1-Lipschitz* if and only if it satisfies

$$|f(\mathbf{m}) - f(\mathbf{n})| \le \|\mathbf{m}-\mathbf{n}\|_1 \text{ for all } \mathbf{m},\mathbf{n} \in \mathbb{Z}^2.$$

Lemma 4.3. *If A is a near-sighted operator acting in $\mathcal{H}_{\mathrm{disc}}$ with range ζ, then $\mathrm{e}^{\pm\lambda f} A \mathrm{e}^{\mp\lambda f}$ is bounded for every $0 \le \lambda < 1/\zeta$ and every 1-Lipschitz function f.*

Proof. For every $\mathbf{m} \in \mathbb{Z}^2$, we compute

$$\begin{aligned}\sum_{\mathbf{n}\in\mathbb{Z}^2} \left|\left(\mathrm{e}^{\pm\lambda f} A \mathrm{e}^{\mp\lambda f}\right)_{\mathbf{m},\mathbf{n}}\right| &= \sum_{\mathbf{n}\in\mathbb{Z}^2} \left|\mathrm{e}^{\pm\lambda f(\mathbf{m})} A_{\mathbf{m},\mathbf{n}} \mathrm{e}^{\mp\lambda f(\mathbf{n})}\right| \\ &= \sum_{\mathbf{n}\in\mathbb{Z}^2} \left|A_{\mathbf{m},\mathbf{n}} \mathrm{e}^{\pm\lambda(f(\mathbf{m})-f(\mathbf{n}))}\right| \\ &\leq C \sum_{\mathbf{n}\in\mathbb{Z}^2} \mathrm{e}^{-\frac{1}{\zeta}\|\mathbf{m}-\mathbf{n}\|_1} \mathrm{e}^{\lambda|f(\mathbf{m})-f(\mathbf{n})|} \\ &\leq C \sum_{\mathbf{n}\in\mathbb{Z}^2} \mathrm{e}^{-\frac{1}{\zeta}\|\mathbf{m}-\mathbf{n}\|_1} \mathrm{e}^{\lambda\|\mathbf{m}-\mathbf{n}\|_1} \\ &= C \sum_{\mathbf{n}\in\mathbb{Z}^2} \mathrm{e}^{-\left(\frac{1}{\zeta}-\lambda\right)\|\mathbf{n}\|_1},\end{aligned}$$

where we have used the near-sightedness of A, the inequality $|\mathrm{e}^a| \leq \mathrm{e}^{|a|}$ for all $a \in \mathbb{R}$, the fact that f is a 1-Lipschitz function and $\mathbb{Z}^2$ is invariant under $\mathbb{Z}^2$-translation. The series on the right-hand side of the last inequality is finite as long as $\lambda < \frac{1}{\zeta}$, so we conclude by invoking Remark 4.1. □

Definition 4.4. Let $A \in \mathcal{B}(\mathcal{H}_{\mathrm{disc}})$. For $j \in \{1, 2\}$ and $\alpha > 0$, we say that A is *α-confined in jth-direction*[7] if and only if

$$A\,\mathrm{e}^{\alpha|X_j|} \text{ is bounded.}$$

Clearly, if A is α-confined in jth-direction for some $\alpha > 0$ and $j \in \{1, 2\}$, then A is λ-confined in jth-direction for every $0 < \lambda \leq \alpha$.

Lemma 4.5. *Let A be a near-sighted operator acting in $\mathcal{H}_{\mathrm{disc}}$, with range ζ, and let Λ_j be a switch function in jth-direction. Then*

$$[\Lambda_j, A] \textit{ is } \alpha\textit{-confined in } j\textit{th-direction,}$$

for all α such that $0 < \alpha < 1/\zeta$.

Proof. For $0 < \alpha < \frac{1}{\zeta}$, one notices that

$$[\Lambda_j, A]\,\mathrm{e}^{\alpha|X_j|} = \Lambda_j A(1-\Lambda_j)\,\mathrm{e}^{\alpha|X_j|} - (1-\Lambda_j)A\Lambda_j\,\mathrm{e}^{\alpha|X_j|}. \tag{4.1}$$

We analyze the first summand on the right-hand side (the second is similarly bounded)

$$\Lambda_j A(1-\Lambda_j)\mathrm{e}^{\alpha|X_j|} = \Lambda_j \mathrm{e}^{-\alpha X_j} \cdot \mathrm{e}^{\alpha X_j} A \mathrm{e}^{-\alpha X_j} \cdot (1-\Lambda_j)\mathrm{e}^{\alpha X_j+\alpha|X_j|} \tag{4.2}$$

The middle term is bounded by Lemma 4.3 since A is near-sighted and the two other terms are bounded due to the support of the switch function. □

Proposition 4.6. *Let $j \neq k \in \{1, 2\}$. If A is α-confined in the jth-direction, B is a bounded operator such that B^* is β-confined in the kth-direction and C is an operator such that*

$$\mathrm{e}^{-\alpha|X_1|} C \mathrm{e}^{\alpha|X_1|} \textit{ is bounded or } \mathrm{e}^{\beta|X_2|} C \mathrm{e}^{-\beta|X_2|} \textit{is bounded,}$$

then ACB is trace class.

[7] In the terminology of [14].

Proof. Without loss of generality, suppose that $j = 1$ and $k = 2$. Assume that $\mathrm{e}^{-\alpha|X_1|} C \mathrm{e}^{\alpha|X_1|}$ is bounded. We have that

$$ACB = A\mathrm{e}^{\alpha|X_1|} \cdot \mathrm{e}^{-\alpha|X_1|} C \mathrm{e}^{\alpha|X_1|} \cdot \mathrm{e}^{-\alpha|X_1|} \mathrm{e}^{-\beta|X_2|} \cdot \mathrm{e}^{\beta|X_2|} B,$$

is trace class. Indeed, on the right-hand side the first and the second factors are bounded by hypotheses. Concerning the fourth factor, in view of $T^*S^* \subseteq (ST)^*$ for any S and T closed, densely defined operators in $\mathcal{H}_{\mathrm{disc}}$, we have $\left\|\mathrm{e}^{\beta|X_2|} B\right\| \leq \left\|\left(B^* \mathrm{e}^{\beta|X_2|}\right)^*\right\| = \left\|B^* \mathrm{e}^{\beta|X_2|}\right\| < \infty$ by hypothesis. The third factor is trace class since it is a positive multiplication operator associated to a summable function.

On the other hand, assume that $\mathrm{e}^{\beta|X_2|} C \mathrm{e}^{-\beta|X_2|}$ is bounded. Writing

$$ACB = A\mathrm{e}^{\alpha|X_1|} \cdot \mathrm{e}^{-\alpha|X_1|} \mathrm{e}^{-\beta|X_2|} \cdot \mathrm{e}^{\beta|X_2|} C \mathrm{e}^{-\beta|X_2|} \cdot \mathrm{e}^{\beta|X_2|} B,$$

we can argue as before and conclude the proof. □

Remark 4.7 (**Discrete versus continuum models**). This strategy to establish trace class property is based on the fact that $\mathrm{e}^{-\alpha|X_1|} \mathrm{e}^{-\beta|X_2|}$ is trace class for some $\alpha, \beta > 0$, a property which holds true for the discrete models considered in this paper, but not for continuum models. In other words, this property is rooted in the underlying ultraviolet cutoff of the discrete models. The generalization to continuum models would require further assumptions on the operators such as localization in energy.

Remark 4.8. One might naively think that $[P, \Lambda_1 S_z]$ is α-confined in the 1st-direction for some $\alpha > 0$, since P is near-sighted (see the forthcoming Lemma 5.1) and S_z acts non-trivially only on the $\mathbb{C}^2$ sector. This guess is not true in general. Indeed, we have

$$[P, \Lambda_1 S_z] = [P, S_z]\Lambda_1 + S_z[P, \Lambda_1].$$

On the right-hand side, the second summand is α-confined in the 1st-direction for all $0 < \alpha < 1/\xi_P$ by Lemma 4.5, while the first summand has no reason to be confined, since $[P, S_z]$ is a priori only a bounded operator which does not have *decreasing properties in space*. Consequently, $\mathcal{G}_K^{s_z}$ is not trace class in general, since it is not confined in the 1st-direction. This is why we had to introduce the directional principal value trace in the definition of $G_K^{s_z}$.

5. Proof of the Main Results

Recall that the Hamiltonian operator H satisfies Assumption 2.2. Namely, H is near-sighted, periodic and with a spectral gap Δ. For $\mu \in \Delta$, $P = \chi_{(-\infty,\mu)}(H)$ is the corresponding Fermi projection. Under these hypotheses, it is well known that

Lemma 5.1 [3,4,28]. *The Fermi projection P is near-sighted.*

We denote the range of P by ζ_P. Note also that $P^{\perp} = \mathbb{1} - P$ is near-sighted.

Lemma 5.2. *If A is a near-sighted operator acting in $\mathcal{H}_{\mathrm{disc}}$, then we have that*

$$[A, X_j] \text{ is bounded for } j \in \{1, 2\}.$$

Proof. For $j = 1$ and fixed $\mathbf{m} \in \mathbb{Z}^2$, we compute

$$\sum_{\mathbf{n}\in\mathbb{Z}^2} \left|([A, X_1])_{\mathbf{m},\mathbf{n}}\right| = \sum_{\mathbf{n}\in\mathbb{Z}^2} |m_1 - n_1| \, |A_{\mathbf{m},\mathbf{n}}| \leq C \sum_{\mathbf{n}\in\mathbb{Z}^2} \mathrm{e}^{-\frac{1}{\zeta}\|\mathbf{m}-\mathbf{n}\|_1} |m_1 - n_1| \,. \tag{5.1}$$

Clearly, the series on the right-hand side is convergent and its limit is independent from $\mathbf{m}$ by the invariance of $\mathbb{Z}^2$ under $\mathbb{Z}^2$-translations. We conclude by using Remark 4.1. □

Lemma 5.3. *If A is a periodic operator acting in $\mathcal{H}_{\mathrm{disc}}$ and S is an operator acting non-trivially on $\mathbb{C}^N \otimes \mathbb{C}^2$ only, then for $j \in \{1, 2\}$ we have the following*

(i) *the operator $[A, X_j]$ is periodic, namely*

$$([A, X_j])_{\mathbf{m},\mathbf{n}} = ([A, X_j])_{\mathbf{m}-\mathbf{p},\mathbf{n}-\mathbf{p}} \quad \textit{for all } \mathbf{m}, \mathbf{n}, \mathbf{p} \in \mathbb{Z}^2;$$

(ii) *the operator $[A, X_j S]$ satisfies*

$$([A, X_j S])_{\mathbf{m},\mathbf{n}} = ([A, X_j S])_{\mathbf{m}-\mathbf{p},\mathbf{n}-\mathbf{p}} - p_j ([A, S])_{\mathbf{m}-\mathbf{p},\mathbf{n}-\mathbf{p}} \quad \textit{for all } \mathbf{m}, \mathbf{n}, \mathbf{p} \in \mathbb{Z}^2.$$

Proof. We use the basis $\delta_{\mathbf{n}}^{(k)} := \delta_{\mathbf{n}} \otimes b_k \in \mathcal{H}_{\mathrm{disc}}$ where $\delta_{\mathbf{n}}$ is defined as usual by $(\delta_{\mathbf{n}})_{\mathbf{m}} = \delta_{\mathbf{n},\mathbf{m}}$ and $\{b_k\}_{k\in\{1,\ldots,2N\}}$ is an orthonormal basis of $\mathbb{C}^N \otimes \mathbb{C}^2$. We denote by $T_{\mathbf{p}}$ the translation operator by the vector $\mathbf{p} \in \mathbb{Z}^2$, acting as

$$(T_{\mathbf{p}}\varphi)_{\mathbf{n}} := \varphi_{\mathbf{n}-\mathbf{p}} \quad \text{for all } \varphi \in \mathcal{H}_{\mathrm{disc}}.$$

(i) By Jacobi identity, we have

$$[[A, X_j], T_{\mathbf{p}}] = -[[T_{\mathbf{p}}, A], X_j] - [[X_j, T_{\mathbf{p}}], A] = -[[X_j, T_{\mathbf{p}}], A] = -p_j [T_{\mathbf{p}}, A] = 0, \tag{5.2}$$

where we have used the periodicity of A and the identity

$$[X_j, T_{\mathbf{p}}] = p_j T_{\mathbf{p}} \quad \text{for all } \mathbf{p} \in \mathbb{Z}^2. \tag{5.3}$$

By the commutation relation (5.2) for every $\mathbf{m}, \mathbf{n}, \mathbf{p} \in \mathbb{Z}^2$, we obtain

$$\begin{aligned} ([A, X_j])_{\mathbf{m},\mathbf{n}}^{(i),(j)} &:= \left\langle \delta_{\mathbf{m}}^{(i)}, [A, X_j] \, \delta_{\mathbf{n}}^{(j)} \right\rangle = \left\langle \delta_{\mathbf{m}}^{(i)}, T_{\mathbf{p}}^* [A, X_j] T_{\mathbf{p}} \delta_{\mathbf{n}}^{(j)} \right\rangle \\ &= \left\langle \delta_{\mathbf{m}-\mathbf{p}}^{(i)}, [A, X_j] \delta_{\mathbf{n}-\mathbf{p}}^{(j)} \right\rangle = ([A, X_j])_{\mathbf{m}-\mathbf{p},\mathbf{n}-\mathbf{p}}^{(i),(j)} \end{aligned}$$

for all $i, j \in \{1, \ldots, 2N\}$.

(ii) By Leibniz rule, we have

$$[A, X_j S] = [A, X_j] S + X_j [A, S]. \tag{5.4}$$

On the right-hand side of the last equation, the first summand is periodic, as it is the product of an operator which is periodic by the previous claim (i) and S, which acts non-trivially only in the sector $\mathbb{C}^N \otimes \mathbb{C}^2$. Instead, the second summand is such that, in view of identity (5.3) and the periodicity of $[A, S]$,

$$[X_j [A, S], T_{\mathbf{p}}] = [X_j, T_{\mathbf{p}}][A, S] = p_j T_{\mathbf{p}} [A, S].$$

Therefore, using decomposition (5.4), the claim (i), the previous relation and the periodicity of $[A, S]$, for every $\mathbf{m}, \mathbf{n}, \mathbf{p} \in \mathbb{Z}^2$ we have

$$\begin{aligned}([A, X_j S])^{(i),(j)}_{\mathbf{m},\mathbf{n}} &= ([A, X_j]S)^{(i),(j)}_{\mathbf{m}-\mathbf{p},\mathbf{n}-\mathbf{p}} \\ &\quad + \left\langle \delta^{(i)}_{\mathbf{m}}, T^*_{\mathbf{p}} X_j [A, S] T_{\mathbf{p}}\, \delta^{(j)}_{\mathbf{n}} \right\rangle - p_j \left\langle \delta^{(i)}_{\mathbf{m}}, [A, S]\, \delta^{(j)}_{\mathbf{n}} \right\rangle \\ &= ([A, X_j S])^{(i),(j)}_{\mathbf{m}-\mathbf{p},\mathbf{n}-\mathbf{p}} - p_j ([A, S])^{(i),(j)}_{\mathbf{m}-\mathbf{p},\mathbf{n}-\mathbf{p}},\end{aligned}$$

for all $i, j \in \{1, \ldots, 2N\}$. □

5.1. Proof of Lemma 2.7

The operator $\mathfrak{T}_{s_z}$ is periodic, since $[P, X_2]$ is so by Lemma 5.3.(i) and the other operators involved in its definition are periodic. It is also bounded as $[P, X_2]$ is so by Lemmas 5.1 and 5.2, and the other operators are bounded. As $\mathfrak{T}_{s_z}$ is periodic and bounded, one concludes by Proposition 3.3. □

5.2. Proof of Theorem 2.8

In view of Lemma 2.7, one has that $\tau(\mathfrak{T}_{s_z})$ is well defined. By algebraic manipulations and Proposition 3.5, one obtains

$$\begin{aligned}\tau(\mathfrak{T}_{s_z}) &= \mathrm{i}\tau(P S_z P^\perp [P, X_2]) + \mathrm{i}\tau(P[P, X_2] P^\perp S_z P) \\ &= \mathrm{i}\tau(S_z P^\perp [P, X_2] P + S_z P [P, X_2] P^\perp) = \mathrm{i}\tau(S_z [P, X_2]) = \mathrm{i}\tau([S_z P, X_2]).\end{aligned}$$

As mentioned above, $S_z[P, X_2] = [S_z P, X_2]$ is a periodic bounded operator. Hence, in view of Propositions 3.1 and 3.3, the commutation relation $[X_2, \chi_1] = 0$ and the identity $\chi_1^2 = \chi_1$, we rewrite the term on the right-hand side of the last equality as

$$\begin{aligned}\mathrm{i}\tau([S_z P, X_2]) &= \mathrm{i}\,\mathrm{Tr}(\chi_1 S_z P \chi_1 X_2 \chi_1) - \mathrm{i}\,\mathrm{Tr}(\chi_1 X_2 \chi_1 S_z P \chi_1) \\ &= \mathrm{i}\,\mathrm{Tr}(\chi_1 S_z P \chi_1 X_2 \chi_1) - \mathrm{i}\,\mathrm{Tr}(\chi_1 S_z P \chi_1 X_2 \chi_1) = 0.\end{aligned}$$

□

5.3. Proof of Theorem 2.9

Part (1) Assume that $G^s_K(\Lambda_1, \Lambda_2)$ (exists and) is finite for a particular switch function Λ_1. Given another switch function Λ_1', we set $\Delta\Lambda_1 = \Lambda_1 - \Lambda_1'$. By algebraic manipulations, using $P^2 = P$ and $P^\perp = \mathbb{1} - P$, we have

$$\begin{aligned}G^s_K(\Delta\Lambda_1, \Lambda_2) &= \text{1-pvTr}\,(\mathrm{i}P[[P, \Delta\Lambda_1 S_z],\, [P, \Lambda_2]]P) \\ &= \text{1-pvTr}\left(\mathrm{i}[P, \Delta\Lambda_1 S_z] P^\perp [P, \Lambda_2] - \mathrm{i}[P, \Lambda_2] P^\perp [P, \Delta\Lambda_1 S_z]\right) \\ &= \text{1-pvTr}\left(\mathrm{i}P \Delta\Lambda_1 S_z P^\perp [P, \Lambda_2] + \mathrm{adj}\right),\end{aligned} \tag{5.5}$$

where adj means that the adjoint of the sum of all operators to the left is added. Notice that $\mathrm{i}P\Delta\Lambda_1 S_z P^\perp [P, \Lambda_2] = \mathrm{i}P\Delta\Lambda_1 S_z [P, \Lambda_2] P$ is trace class by Proposition 4.6, and so is its adjoint. Indeed, $\Delta\Lambda_1$ is compactly supported; thus in particular, it is confined in the 1st-direction and $[P, \Lambda_2]$ is confined in the 2nd-direction by Lemma 4.5. So the 1-pvTr(·) can be replaced by Tr(·). Moreover, each term is separately trace class so we split the trace and use cyclicity on each term. We end up with

$$\begin{aligned} G_K^{s_z}(\Delta\Lambda_1, \Lambda_2) &= \mathrm{i}\,\mathrm{Tr}\left(\Delta\Lambda_1 S_z P \Lambda_2 P^\perp\right) - \mathrm{i}\,\mathrm{Tr}\left(\Delta\Lambda_1 S_z P^\perp \Lambda_2 P\right) \\ &= \mathrm{i}\,\mathrm{Tr}\left(\Delta\Lambda_1 S_z [P, \Lambda_2]\right) \\ &= \mathrm{i} \sum_{\mathbf{m}\in\mathbb{Z}^2} \mathrm{tr}\,\big(\Delta\Lambda_1(m_1) S_z \Lambda_2(m_2) P_{\mathbf{m},\mathbf{m}} \\ &\quad - \Delta\Lambda_1(m_1) S_z P_{\mathbf{m},\mathbf{m}} \Lambda_2(m_2)\big) \\ &= 0. \end{aligned}$$

Part (2) Equation (2.4) is implied by Lemma 5.3.(ii). Once established (2.4), Proposition 3.4 yields the proof of Part (2).

Part (3) We introduce the function

$$\Xi(n_1) = \begin{cases} 0 & \text{if } n_1 < -1/2, \\ n_1 + 1/2 & \text{if } -1/2 \le n_1 < 1/2 \\ 1 & \text{if } n_1 \ge 1/2, \end{cases} \tag{5.6}$$

which interpolates linearly in the interval $|n_1| \le 1/2$ and, for $l > 0$ we define the functions $\Xi^{(l)}(n_1) := \Xi(\frac{n_1}{l})$ which have slope $1/l$ in the interval $|n_1| \le l/2$. Now, we define the *approximate position functions* in the 1st-direction as

$$X_1^{(l)} := l\left(\Xi^{(l)} - \frac{1}{2}\right) \quad \text{such that}$$

$$X_1^{(l)}(n_1) = \begin{cases} -l/2 & \text{if } n_1 < -l/2, \\ n_1 & \text{if } -l/2 \le n_1 < l/2 \\ l/2 & \text{if } n_1 \ge l/2. \end{cases} \tag{5.7}$$

Notice that for every $l > 0$ the functions $\Xi^{(l)}$ are particular switch functions in the 1st-direction.

We now compute $G_K^{s_z}(\Xi^{(l)}, \Lambda_2)$ and show that it is finite. In view of Part (1), this fact will imply that $G_K^{s_z}(\Lambda_1, \Lambda_2)$ is finite for every switch function Λ_1, and independent of the choice of the latter. Notice that

$$G_K^{s_z}\big(\Xi^{(l)}, \Lambda_2\big) = \frac{1}{l} G_K^{s_z}\big(X_1^{(l)}, \Lambda_2\big) + \frac{1}{2} G_K^{s_z}\big(\mathbb{1}, \Lambda_2\big), \tag{5.8}$$

provided the two summands separately exist and are finite (which is what we are going to prove).

We focus attention on the first summand on the right-hand side of the last equation. Recall that, by definition (1.4), one has

$$G_K^{s_z}\big(X_1^{(l)}, \Lambda_2\big) = 1\text{-pvTr}\big(\mathcal{G}_K^{s_z}\big(X_1^{(l)}, \Lambda_2\big)\big)$$

where

$$\mathcal{G}_K^{s_z}\big(X_1^{(l)}, \Lambda_2\big) = \mathrm{i}P[[P, X_1^{(l)} S_z],\, [P, \Lambda_2]]P.$$

We analyze $\mathcal{G}_K^{s_z}\big(X_1^{(l)}, \Lambda_2\big)$. By algebraic manipulations, we obtain

$$\begin{aligned}\mathcal{G}_K^{s_z}\big(X_1^{(l)}, \Lambda_2\big) &= \mathrm{i}[P, X_1^{(l)} S_z] P^\perp [P, \Lambda_2] - \mathrm{i}[P, \Lambda_2] P^\perp [P, X_1^{(l)} S_z] \\ &= \underbrace{\mathrm{i}[P, X_1^{(l)}] S_z P^\perp [P, \Lambda_2]}_{=:\mathcal{G}_{K,a}^{s_z}} + \underbrace{X_1^{(l)} \mathrm{i}[P, S_z] P^\perp [P, \Lambda_2]}_{=:\mathcal{G}_{K,b}^{s_z}} + \mathrm{adj}. \end{aligned} \tag{5.9}$$

By Proposition 4.6 and Lemma 4.5, $[P, X_1^{(l)}] S_z [P, \Lambda_2]$ is trace class, and since P is bounded $\mathcal{G}_{K,a}^{s_z}\big(X_1^{(l)}, \Lambda_2\big)$ is trace class, as well as its adjoint. Thus by Lemma 3.2, $1\text{-pvTr}\big(\mathcal{G}_{K,a}^{s_z}\big(X_1^{(l)}, \Lambda_2\big) + \mathrm{adj}\big) = \mathrm{Tr}\,\big(\mathcal{G}_{K,a}^{s_z}\big(X_1^{(l)}, \Lambda_2\big) + \mathrm{adj}\big)$.

As explained in "Appendix B," for periodic operators the trace of an expression involving switch functions may become a trace on the unit cell where position operators replace commutators with switch functions. In particular, by Lemma B.3 we obtain

$$\begin{aligned}\frac{1}{l}\,\mathrm{Tr}\,\big(\mathcal{G}_{K,a}^{s_z}\big(X_1^{(l)}, \Lambda_2\big) + \mathrm{adj}\big) &= \frac{1}{l}\,\mathrm{Tr}\,\big(\mathrm{i}[P, X_1^{(l)}] S_z P^\perp [P, \Lambda_2] + \mathrm{adj}\big) \\ &= \mathrm{Tr}\,\big(\mathrm{i}[P, \Xi^{(l)}] S_z P^\perp [P, \Lambda_2] + \mathrm{adj}\big) \\ &= \mathrm{Tr}(-\chi_1 \mathrm{i} P X_1 S_z P^\perp X_2 P \chi_1 + \mathrm{adj}) \\ &= \mathrm{Tr}(\chi_1 \mathrm{i} P [[P, X_1 S_z], [P, X_2]] P \chi_1).\end{aligned}$$

Finally, by Part (2) and by the last equation we obtain that[8]

$$\frac{1}{l}\,\mathrm{Tr}\,\big(\mathcal{G}_{K,a}^{s_z}\big(X_1^{(l)}, \Lambda_2\big) + \mathrm{adj}\big) = \tau(\mathrm{i}P[[P, X_1 S_z], [P, X_2]]P) = \sigma_K^{s_z}. \tag{5.10}$$

Now, we compute $1\text{-pvTr}\big(\mathcal{G}_{K,b}^{s_z} + \mathrm{adj}\big)$, whose argument is defined in Eq. (5.9). Notice that $\chi_{1,L} \mathcal{G}_{K,b}^{s_z} \chi_{1,L}$, as well as its adjoint, is trace class by Proposition 4.6 since $[P, \Lambda_2]$ is confined in the 2nd-direction and $\chi_{1,L}$ is trivially confined in the 1st-one.

By Lemma B.2, we obtain

$$\begin{aligned}\mathrm{Tr}\,\big(\chi_{1,L} \mathcal{G}_{K,b}^{s_z} \chi_{1,L} + \mathrm{adj}\big) &= \mathrm{Tr}\,\big(- \chi_{1,L} X_1^{(l)} \mathrm{i}[P, S_z] P^\perp X_2 P \chi_{2,1} \chi_{1,L} + \mathrm{adj}\big) \\ &= \mathrm{Tr}\,\big(\chi_{1,L} X_1^{(l)} \mathrm{i}[P, S_z] P^\perp [P, X_2] \chi_{2,1} \chi_{1,L}\big) + \\ &\quad - \mathrm{Tr}\,\big(\chi_{1,L} \chi_{2,1} [P, X_2] P^\perp \mathrm{i}[P, S_z] X_1^{(l)} \chi_{1,L}\big).\end{aligned} \tag{5.11}$$

The two operators in the argument of the trace are trace class by similar argument as above. Thus, as $\chi_{2,1}$ squares to itself, by using Proposition 3.1 we obtain

$$\begin{aligned}&\mathrm{Tr}\,\big(\chi_{1,L} X_1^{(l)} \mathrm{i}[P, S_z] P^\perp [P, X_2] \chi_{2,1} \chi_{1,L}\big) \\ &\quad = \mathrm{Tr}\,\big(\chi_{1,L} \chi_{2,1} X_1^{(l)} \mathrm{i}[P, S_z] P^\perp [P, X_2] \chi_{2,1} \chi_{1,L}\big).\end{aligned} \tag{5.12}$$

[8]Notice that we do not need to consider the limit $l \to +\infty$, as one might expect.

Similarly, using also that multiplicative operators by position functions commute, we obtain

$$\begin{aligned}&\operatorname{Tr}\big(\chi_{1,L}\chi_{2,1}[P,X_2]P^{\perp}\mathrm{i}[P,S_z]X_1^{(l)}\chi_{1,L}\big)\\&\quad=\operatorname{Tr}\big(\chi_{1,L}\chi_{2,1}X_1^{(l)}[P,X_2]P^{\perp}\mathrm{i}[P,S_z]\chi_{2,1}\chi_{1,L}\big).\end{aligned}\tag{5.13}$$

Therefore, plugging (5.12) and (5.13) into equation (5.11), we have

$$\begin{aligned}\operatorname{Tr}\big(\chi_{1,L}\mathcal{G}^{s_z}_{K,b}\chi_{1,L}+\mathrm{adj}\big)&=\operatorname{Tr}\big(\chi_{1,L}\chi_{2,1}X_1^{(l)}\mathrm{i}P[[P,S_z],[P,X_2]]P\chi_{2,1}\chi_{1,L}\big)\\&=\operatorname{Tr}\big(\chi_{1,L}\chi_{2,1}X_1^{(l)}\mathcal{T}_{s_z}\chi_{2,1}\chi_{1,L}\big).\end{aligned}$$

Observe that for every fixed $L\in 2\mathbb{N}+1$, the operator $\chi_{1,L}\chi_{2,1}X_1^{(l)}\mathcal{T}_{s_z}\chi_{2,1}\chi_{1,L}$ is trace class, as $\chi_{1,L}\chi_{2,1}$ is trace class for the previous analysis and $\mathcal{T}_{s_z}$ is bounded by Lemma 2.7. We compute its trace through the diagonal kernel, using Lemma 2.7,

$$\begin{aligned}\operatorname{Tr}\big(\chi_{1,L}\chi_{2,1}X_1^{(l)}\mathcal{T}_{s_z}\chi_{2,1}\chi_{1,L}\big)&=\sum_{\substack{m_1\in\mathbb{Z}\\|m_1|\le L/2}}X_1^{(l)}(m_1)\operatorname{tr}\big((\mathcal{T}_{s_z})_{(m_1,0),(m_1,0)}\big)\\&=\sum_{\substack{m_1\in\mathbb{Z}\\|m_1|\le L/2}}X_1^{(l)}(m_1)\operatorname{tr}\big((\mathcal{T}_{s_z})_{\mathbf{0},\mathbf{0}}\big)\\&=\tau(\mathcal{T}_{s_z})\sum_{\substack{m_1\in\mathbb{Z}\\|m_1|\le L/2}}X_1^{(l)}(m_1)\equiv 0,\end{aligned}\tag{5.14}$$

as the function $X_1^{(l)}(m_1)$ is odd and the interval $|m_1|\le L/2$ is symmetric with respect to 0. (We could also invoke the fact that $\tau(\mathcal{T}_{s_z})=0$ by Theorem 2.8). Thus,

$$1\text{-pvTr}\big(\mathcal{G}^{s_z}_{K,b}+\mathrm{adj}\big)=0.\tag{5.15}$$

Using Eqs. (5.10) and (5.15), we obtain

$$\frac{1}{l}1\text{-pvTr}\big(\mathcal{G}^{s_z}_K\big(X_1^{(l)},\Lambda_2\big)\big)=\sigma^{s_z}_K+0=\sigma^{s_z}_K.\tag{5.16}$$

Now, we focus attention on the second summand on the right-hand side of (5.8). We have

$$\frac{1}{2}G^{s_z}_K\big(\mathbb{1},\Lambda_2\big)=\frac{1}{2}\lim_{\substack{L\to\infty\\L\in 2\mathbb{N}+1}}\operatorname{Tr}(\chi_{1,L}\mathrm{i}P[[P,S_z],\,[P,\Lambda_2]]P\chi_{1,L}).\tag{5.17}$$

Notice that $\chi_{1,L}\mathrm{i}P[[P,S_z],\,[P,\Lambda_2]]P\chi_{1,L}$ is trace class, as one proves by applying Proposition 4.6 and arguing as in the previous cases.

By Lemma B.2, the identity $\chi_{2,1}^2=\chi_{2,1}$ and Proposition 3.1, we obtain

$$\begin{aligned}\operatorname{Tr}(\chi_{1,L}\mathrm{i}P[[P,S_z],\,[P,\Lambda_2]]P\chi_{1,L})&=-\operatorname{Tr}(\chi_{1,L}\mathrm{i}[P,S_z]P^{\perp}X_2P\chi_{2,1}\chi_{1,L})+\\&\quad-\operatorname{Tr}(\chi_{1,L}\chi_{2,1}PX_2P^{\perp}\mathrm{i}[P,S_z]\chi_{1,L})\\&=\operatorname{Tr}(\chi_{1,L}\chi_{2,1}\mathcal{T}_{s_z}\chi_{2,1}\chi_{1,L}).\end{aligned}\tag{5.18}$$

As $\chi_{1,L}\chi_{2,1}\mathfrak{T}_{s_z}\chi_{2,1}\chi_{1,L}$ is trace class, computing its trace via diagonal kernel and using Lemma 2.7, we get

$$\begin{aligned}\operatorname{Tr}(\chi_{1,L}\chi_{2,1}\mathfrak{T}_{s_z}\chi_{2,1}\chi_{1,L}) &= \sum_{\substack{m_1\in\mathbb{Z}\\|m_1|\le L/2}} \operatorname{tr}((\mathfrak{T}_{s_z})_{(m_1,0),(m_1,0)}) \\ &= \sum_{\substack{m_1\in\mathbb{Z}\\|m_1|\le L/2}} \operatorname{tr}((\mathfrak{T}_{s_z})_{\mathbf{0},\mathbf{0}}) = \sum_{\substack{m_1\in\mathbb{Z}\\|m_1|\le L/2}} \tau(\mathfrak{T}_{s_z}).\end{aligned}$$

Thus, plugging the last equality and Eq. (5.18) in (5.17), we obtain

$$\frac{1}{2}G_K^{s_z}\left(\mathbb{1},\Lambda_2\right) = \frac{1}{2}\lim_{\substack{L\to\infty\\L\in 2\mathbb{N}+1}} \sum_{\substack{m_1\in\mathbb{Z}\\|m_1|\le L/2}} \tau(\mathfrak{T}_{s_z}) = 0 \tag{5.19}$$

in view of Theorem 2.8. □

It is worthwhile to notice that, without using Theorem 2.8, by plugging equalities (5.16) and (5.19) into (5.8), one would obtain

$$\begin{aligned}G_K^{s_z}(\Xi^{(l)},\Lambda_2) &= \frac{1}{l}G_K^{s_z}\left(X_1^{(l)},\Lambda_2\right) + \frac{1}{2}G_K^{s_z}\left(\mathbb{1},\Lambda_2\right) \\ &= \sigma_K^{s_z} + \frac{1}{2}\lim_{\substack{L\to\infty\\L\in 2\mathbb{N}+1}} \sum_{\substack{m_1\in\mathbb{Z}\\|m_1|\le L/2}} \tau(\mathfrak{T}_{s_z}).\end{aligned} \tag{5.20}$$

As remarked in Sect. 2, the second summand on the right-hand side is either zero, if $\tau(\mathfrak{T}_{s_z}) = 0$, or diverging to $\pm\infty$. Hence, the equality of (the Kubo-like terms of) the spin conductance and spin conductivity is rooted in the fact that the spin-torque response $\tau(\mathfrak{T}_{s_z})$ vanishes on the mesoscopic scale. We expect that such a physically relevant condition will play a role also in a more general setting.

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Appendix A: The Kane–Mele Model in First Quantization Formalism

In this appendix, we review an explicit model that satisfies Assumption 2.2 and where spin is not conserved. This model was first introduced by Kane and Mele [25, 26]. Here, we propose a first quantized formulation of it, but first we discuss the dimerization method mentioned at the beginning of Sect. 2.

A.1. The Honeycomb Structure

The model describes independent electrons on a honeycomb structure $\mathcal{C}$, illustrated in Fig. 1. The structure is characterized by the *displacement vectors*

$$\mathbf{d}_1 = d\begin{pmatrix}\frac{1}{2} & -\frac{\sqrt{3}}{2}\end{pmatrix}, \quad \mathbf{d}_2 = d\begin{pmatrix}\frac{1}{2} & \frac{\sqrt{3}}{2}\end{pmatrix}, \quad \mathbf{d}_3 = d\begin{pmatrix}-1 & 0\end{pmatrix} = -\mathbf{d}_1 - \mathbf{d}_2,$$

where d is the smallest distance between two points of $\mathcal{C}$, which generate the *periodicity vectors*

$$\mathbf{a}_1 = \mathbf{d}_2 - \mathbf{d}_3, \quad \mathbf{a}_2 = \mathbf{d}_3 - \mathbf{d}_1, \quad \mathbf{a}_3 = \mathbf{d}_1 - \mathbf{d}_2 = -\mathbf{a}_1 - \mathbf{a}_2. \tag{A.1}$$

The vectors $\mathbf{a}_i$ generate a Bravais lattice $\Gamma := \mathrm{Span}_{\mathbb{Z}}\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\} \cong \mathbb{Z}^2$ where one $\mathbf{a}_i$ is redundant as it is integer linear combination of the two others. Then, any site of the crystal can be reached by a Bravais lattice vector and the use of one of the $\mathbf{d}_i$ vectors. It is then sufficient to pick two $\mathbf{a}_i$-vectors and one $\mathbf{d}_i$-vector to generate the whole crystal. This choice, which is often called a *dimerization* of $\mathcal{C}$, is not unique, as illustrated in Fig. 2.

The above procedure is equivalent to the choice of a periodicity cell that contains two non-equivalent sites A and B (black and white dots in Fig. 1), described as internal degrees of freedom besides the Bravais lattice. Hence, each choice of unit cell provides an isomorphism $\ell^2(\mathcal{C}) \cong \ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^2$, leading to the Hilbert space $\mathcal{H}_{\mathrm{disc}}$ (for $N = 2$) discussed in Sect. 2, when the spin is taken into account.

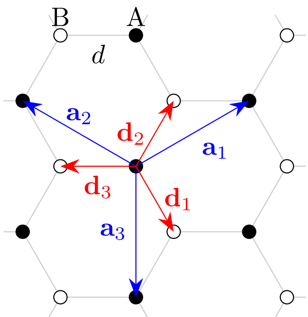

FIGURE 1. The honeycomb structure

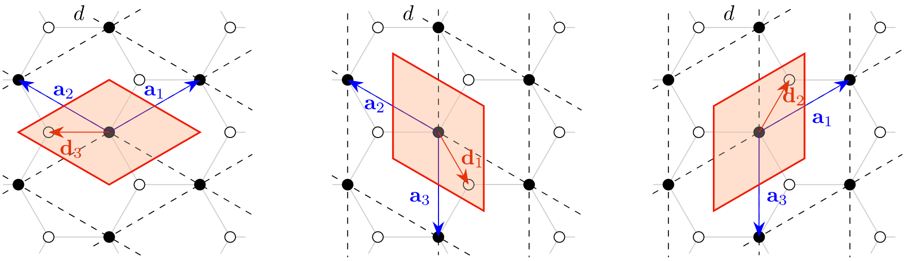

Figure 2. Three possible dimerizations of the honeycomb structure

A.2. The Hamiltonian

The Kane–Mele model is defined, in a first quantization formalism, by the Hamiltonian H_{KM}, acting on $\ell^2(\mathcal{C}) \otimes \mathbb{C}^2$ as

$$H_{\mathrm{KM}} = tH_{\mathrm{NN}} + \lambda_v H_v + \lambda_{\mathrm{SO}} H_{\mathrm{SO}} + \lambda_{\mathrm{R}} H_{\mathrm{R}}$$

where t, $\lambda_v, \lambda_{\mathrm{SO}}$ and λ_{R} are real parameters corresponding to various physical effects. The first term is a nearest-neighbor hopping term:

$$H_{\mathrm{NN}} = \sum_{i=1}^{3} (T_{\mathbf{d}_i} + T_{-\mathbf{d}_i}) \otimes \mathbb{1}_{\mathbb{C}^2}$$

where $T_{\mathbf{u}}$ is a translation operator along vector $\mathbf{u}$, namely

$$(T_{\mathbf{u}}\psi)_{\mathbf{x}} = \begin{cases} \psi_{\mathbf{x}-\mathbf{u}} & \text{if } \mathbf{x} - \mathbf{u} \in \mathcal{C} \\ 0 & \text{otherwise} \end{cases} \quad \text{for all } \psi \in \ell^2(\mathcal{C}) \otimes \mathbb{C}^2.$$

The second term is a sublattice potential that distinguishes sites A and B, namely

$$H_v = (\chi_A - \chi_B) \otimes \mathbb{1}_{\mathbb{C}^2}$$

for χ_A (resp. χ_B) the characteristic function on the sublattice A (resp. sublattice B) of $\mathcal{C}$. The third term is a spin-orbit term, corresponding to an effective and spin-dependent magnetic field due to an electric field inside the two-dimensional crystal. This is a next-to-nearest-neighbor term given by

$$H_{\mathrm{SO}} = -\mathrm{i}\,(\chi_A - \chi_B) \sum_{i=1}^{3} (T_{\mathbf{a}_i} - T_{-\mathbf{a}_i}) \otimes s_z.$$

Finally, the last term is called a Rashba term. This is also a spin-orbit effect but due to an electric field orthogonal to the sample (for example in a heterostructure). This is a nearest-neighbor term given by

$$\begin{aligned} H_{\mathrm{R}} = \mathrm{i}\big(T_{\mathbf{d}_1} - T_{-\mathbf{d}_1}\big) \otimes \left(-\frac{\sqrt{3}s_x + s_y}{2}\right) \\ + \mathrm{i}\big(T_{\mathbf{d}_2} - T_{-\mathbf{d}_2}\big) \otimes \left(\frac{\sqrt{3}s_x - s_y}{2}\right) + \mathrm{i}\big(T_{\mathbf{d}_3} - T_{-\mathbf{d}_3}\big) \otimes s_y \end{aligned}$$

Notice that this last term satisfies $[H_{\mathrm{R}}, S_z] \neq 0$ so that S_z and H_{KM} do not commute whenever $\lambda_R \neq 0$. Moreover, note that H_{KM} is Γ-periodic, since $[T_{\mathbf{u}_1}, T_{\mathbf{u}_2}] = 0$ for any vectors $\mathbf{u}_1$ and $\mathbf{u}_2$, and χ_A and χ_B are Γ-periodic. Thus, H_{KM} commutes with all the translation of the Bravais lattice T_γ for $\gamma \in \Gamma$. It has been shown in [25] that H_{KM} has a spectral gap for a wide region in parameter space, including $\lambda_R \neq 0$ (Figure 1 in [25]).

In summary, H_{KM} is made of on-site (H_v), nearest-neighbor (H_{NN} and H_{R}) and next-to-nearest-neighbor (H_{SO}) terms. Note that after the dimerization procedure a nearest-neighbor term acts on internal degree of freedom, whereas next-to-nearest-neighbor exchange becomes simply nearest-neighbor. Thus, whatever the dimerization, one has

$$(H_{\mathrm{KM}})_{\mathbf{m},\mathbf{n}} = 0 \quad \text{for} \quad \|\mathbf{m} - \mathbf{n}\|_1 > 1$$

so that H_{KM} is trivially near-sighted.

Appendix B: From Switch Functions to Position Operators

In this appendix, we re-elaborate some ideas and techniques which originally appeared in [7] in the continuum case ($\mathbb{R}^2$-covariant Schrödinger operators on the plane). We adapt their proof to the discrete case considered in this paper.

The crucial property of any switch function is the following one.

Lemma B.1. *Let Λ_j be a switch function in the* jth-*direction for $j \in \{1, 2\}$. Then, for every $n \in \mathbb{Z}$ one has*

$$\sum_{m \in \mathbb{Z}} (\Lambda_j(m+n) - \Lambda_j(m)) = n.$$

Proof. For $n = 0$, the claim is trivial. Consider $n \geq 1$. Notice that the summand $\Lambda_j(m+n) - \Lambda_j(m)$ is nonzero only for finitely many $m \in \mathbb{Z}$. Hence,

$$\begin{aligned}\sum_{m \in \mathbb{Z}} (\Lambda_j(m+n) - \Lambda_j(m)) &= \sum_{m \in \mathbb{Z}} \sum_{p=0}^{n-1} \big(\Lambda_j(m + (n-p)) - \Lambda_j(m + (n-p-1))\big) \\ &= \sum_{p=0}^{n-1} \sum_{m \in \mathbb{Z}} \big(\Lambda_j(m) - \Lambda_j(m-1)\big).\end{aligned} \tag{B.1}$$

Notice that $\sum_{m \in \mathbb{Z}} \big(\Lambda_j(m) - \Lambda_j(m-1)\big) = 1$, since there is one and only one point $m \in \mathbb{Z}$ where the summand is not zero. This proves the statement for $n \geq 1$. The proof for $n \leq -1$ is analogous. □

For the sake of clarity, we recall that $\chi_{2,1}$ and χ_1 are characteristic functions, respectively, of the line $\big\{\mathbf{m} \in \mathbb{Z}^2 \colon m_2 = 0\big\}$ and of the point $\{\mathbf{0}\}$.

Lemma B.2. *Let A, B and C be operators in $\mathcal{B}(\mathcal{H}_{\mathrm{disc}})$ which are periodic in the* 2nd-*direction, and let Λ_2 be a switch function in the* 2nd-*direction. If*

$A[B,\Lambda_2]C$ is trace class, A is α-confined in the 1st-*direction, C^* is β-confined in the* 1st-*direction and B satisfies*

$$\mathcal{M}_B := \max\left(\sup_{\mathbf{m}\in\mathbb{Z}^2}\sum_{n_1\in\mathbb{Z}}\left|B_{\mathbf{m},(n_1,0)}m_2\right|, \sup_{n_1\in\mathbb{Z}}\sum_{\mathbf{m}\in\mathbb{Z}^2}\left|B_{\mathbf{m},(n_1,0)}m_2\right|\right) < \infty, \quad \text{(B.2)}$$

then

$$\operatorname{Tr}(A[B,\Lambda_2]C) = -\operatorname{Tr}(AX_2B\chi_{2,1}C).$$

Proof. Since $A[B,\Lambda_2]C$ is trace class, its trace can be computed through the diagonal kernel, and in view of the boundedness of A, $[B,\Lambda_2]$ and C, one has

$$\operatorname{Tr}(A[B,\Lambda_2]C) = \sum_{\mathbf{m}\in\mathbb{Z}^2}\sum_{\mathbf{n}\in\mathbb{Z}^2}\sum_{\mathbf{p}\in\mathbb{Z}^2}\operatorname{tr}\left(A_{\mathbf{m},\mathbf{n}}B_{\mathbf{n},\mathbf{p}}(\Lambda_2(p_2)-\Lambda_2(n_2))C_{\mathbf{p},\mathbf{m}}\right). \quad \text{(B.3)}$$

We will show that the function

$$\left(\mathbb{Z}^2\right)^3 \ni (\mathbf{m},\mathbf{n},\mathbf{p}) \mapsto \operatorname{tr}\left(A_{\mathbf{m},\mathbf{n}}B_{\mathbf{n},\mathbf{p}}(\Lambda_2(p_2)-\Lambda_2(n_2))C_{\mathbf{p},\mathbf{m}}\right) \text{ is in } \ell^1\left(\left(\mathbb{Z}^2\right)^3\right). \quad \text{(B.4)}$$

Thus, we can apply Fubini's Theorem and implement the change of variables $\mathbf{m'} = \mathbf{m} - (0,p_2)$, $\mathbf{n'} = \mathbf{n} - (0,p_2)$. By Lemma B.1 and periodicity in the 2nd-direction, we get that the right-hand side term of (B.3) reads

$$\begin{aligned}\sum_{p_1\in\mathbb{Z}}\sum_{\mathbf{m'}\in\mathbb{Z}^2}\sum_{\mathbf{n'}\in\mathbb{Z}^2}&\operatorname{tr}\left(A_{\mathbf{m'},\mathbf{n'}}B_{\mathbf{n'},(p_1,0)}(-n'_2)C_{(p_1,0),\mathbf{m'}}\right)\\ &= -\sum_{\mathbf{m'}\in\mathbb{Z}^2}\operatorname{tr}\left((AX_2B\chi_{2,1}C)_{\mathbf{m'},\mathbf{m'}}\right).\end{aligned}$$

Observe that by hypothesis (B.2) and Remark 4.1, $X_2B\chi_{2,1}$ is bounded and thus $AX_2B\chi_{2,1}C$ is trace class, as $\chi_{2,1}C \in \mathcal{B}_1(\mathcal{H}_{\mathrm{disc}})$ by Proposition 4.6. Therefore, one concludes that

$$\begin{aligned}\operatorname{Tr}(A[B,\Lambda_2]C) &= -\sum_{\mathbf{m'}\in\mathbb{Z}^2}\operatorname{tr}\left((AX_2B\chi_{2,1}C)_{\mathbf{m'},\mathbf{m'}}\right)\\ &= -\operatorname{Tr}(AX_2B\chi_{2,1}C).\end{aligned}$$

It remains to check (B.4). In view of the equivalence of norms on finite-dimensional vector spaces, one has $|\operatorname{tr}(M)| \leq D_1|M|$ for every matrix M and some $D_1 > 0$. Then by the periodicity in the 2nd-direction, one notices that

$$\begin{aligned}&\sum_{\mathbf{m}\in\mathbb{Z}^2}\sum_{\mathbf{n}\in\mathbb{Z}^2}\sum_{\mathbf{p}\in\mathbb{Z}^2}\left|\operatorname{tr}\left(A_{\mathbf{m},\mathbf{n}}B_{\mathbf{n},\mathbf{p}}(\Lambda_2(p_2)-\Lambda_2(n_2))C_{\mathbf{p},\mathbf{m}}\right)\right|\\ &\quad\leq \frac{D_1}{2}\sum_{\mathbf{m}\in\mathbb{Z}^2}\sum_{\mathbf{n}\in\mathbb{Z}^2}\sum_{\mathbf{p}\in\mathbb{Z}^2}|B_{\mathbf{n},\mathbf{p}}|\,|(\Lambda_2(p_2)-\Lambda_2(n_2))|\left(|A_{\mathbf{m},\mathbf{n}}|^2+|C_{\mathbf{p},\mathbf{m}}|^2\right)\\ &\quad\leq \frac{D_1}{2}\sum_{\mathbf{n}\in\mathbb{Z}^2}\sum_{\mathbf{m'}\in\mathbb{Z}^2}\sum_{\mathbf{p'}\in\mathbb{Z}^2}\left|B_{(n_1,0),\mathbf{p'}}\right|\left|(\Lambda_2(p'_2+n_2)-\Lambda_2(n_2))\right|\left|A_{\mathbf{m'},(n_1,0)}\right|^2\\ &\qquad+\frac{D_1}{2}\sum_{\mathbf{p}\in\mathbb{Z}^2}\sum_{\mathbf{m'}\in\mathbb{Z}^2}\sum_{\mathbf{n'}\in\mathbb{Z}^2}\left|B_{\mathbf{n'},(p_1,0)}\right|\left|(\Lambda_2(p_2)-\Lambda_2(n'_2+p_2))\right|\left|C_{(p_1,0),\mathbf{m'}}\right|^2.\end{aligned}$$

By using Lemma B.1 and exploiting hypotheses on A, B and C one concludes that the above series converge; hence, (B.4) is proven. □

Lemma B.3. *Let A, B and C be periodic operators in $\mathcal{B}(\mathcal{H}_{\mathrm{disc}})$. Let Λ_1, Λ_2 be two switch functions, respectively, in the* 1st *and* 2nd-*direction. If $[A,\Lambda_1]B[C,\Lambda_2]$ is trace class, and A and C satisfy*

$$\sum_{\mathbf{n}\in\mathbb{Z}^2} |A_{0,\mathbf{n}} n_1| < \infty, \qquad \sum_{\mathbf{m}\in\mathbb{Z}^2} |C_{\mathbf{m},0} m_2| < \infty, \tag{B.5}$$

then

$$\mathrm{Tr}([A,\Lambda_1]B[C,\Lambda_2]) = -\,\mathrm{Tr}(\chi_1 A X_1 B X_2 C \chi_1).$$

Proof. Since $[A,\Lambda_1]B[C,\Lambda_2]$ is trace class, its trace can be computed through the diagonal kernel, and in view of boundedness of $[A,\Lambda_1]$, B and $[C,\Lambda_2]$, one has

$$\begin{aligned}&\mathrm{Tr}\Big([A,\Lambda_1]B[C,\Lambda_2]\Big)\\ &\quad= \sum_{\mathbf{m}\in\mathbb{Z}^2}\sum_{\mathbf{n}\in\mathbb{Z}^2}\sum_{\mathbf{p}\in\mathbb{Z}^2} \mathrm{tr}\left(A_{\mathbf{m},\mathbf{n}}(\Lambda_1(n_1)-\Lambda_1(m_1))B_{\mathbf{n},\mathbf{p}}C_{\mathbf{p},\mathbf{m}}(\Lambda_2(m_2)-\Lambda_1(p_2))\right).\end{aligned}$$

Performing the change of variables $\mathbf{n}' = \mathbf{n}-\mathbf{m}$, $\mathbf{p}' = \mathbf{p}-\mathbf{m}$ and using the periodicity, one can rewrite the right-hand side term of the last equation as

$$\begin{aligned}&\sum_{\mathbf{m}\in\mathbb{Z}^2}\sum_{\mathbf{n}'\in\mathbb{Z}^2}\sum_{\mathbf{p}'\in\mathbb{Z}^2} \mathrm{tr}\left(A_{\mathbf{m},\mathbf{n}'+\mathbf{m}}(\Lambda_1(n_1'+m_1)-\Lambda_1(m_1))\right.\\ &\qquad \left.\cdot B_{\mathbf{n}'+\mathbf{m},\mathbf{p}'+\mathbf{m}}C_{\mathbf{p}'+\mathbf{m},\mathbf{m}}(\Lambda_2(m_2)-\Lambda_1(p_2'+m_2))\right)\\ &\qquad = \sum_{\mathbf{m}\in\mathbb{Z}^2}\sum_{\mathbf{n}'\in\mathbb{Z}^2}\sum_{\mathbf{p}'\in\mathbb{Z}^2} \mathrm{tr}\left(A_{\mathbf{0},\mathbf{n}'}(\Lambda_1(n_1'+m_1)-\Lambda_1(m_1))\right.\\ &\qquad \left.\cdot B_{\mathbf{n}',\mathbf{p}'}C_{\mathbf{p}',\mathbf{0}}(\Lambda_2(m_2)-\Lambda_1(p_2'+m_2))\right).\end{aligned} \tag{B.6}$$

By applying Fubini's Theorem and Lemma B.1, one can rewrite the right-hand side

$$\sum_{\mathbf{n}'\in\mathbb{Z}^2}\sum_{\mathbf{p}'\in\mathbb{Z}^2} \mathrm{tr}\left(A_{\mathbf{0},\mathbf{n}'}n_1' B_{\mathbf{n}',\mathbf{p}'}(-p_2')C_{\mathbf{p}',\mathbf{0}}\right) = -\sum_{\mathbf{m}\in\mathbb{Z}^2}\mathrm{tr}\left((\chi_1 A X_1 B X_2 C\chi_1)_{\mathbf{m},\mathbf{m}}\right).$$

Observe that by hypothesis (B.5) and Remark 4.1, $\chi_1 A X_1$ and $X_2 C \chi_1$ are bounded, and thus, $\chi_1 A X_1 B X_2 C \chi_1$ is trace class. Therefore, one concludes that

$$\begin{aligned}\mathrm{Tr}\Big([A,\Lambda_1]B[C,\Lambda_2]\Big) &= -\sum_{\mathbf{m}\in\mathbb{Z}^2}\mathrm{tr}\left((\chi_1 A X_1 B X_2 C\chi_1)_{\mathbf{m},\mathbf{m}}\right)\\ &= -\,\mathrm{Tr}(\chi_1 A X_1 B X_2 C\chi_1).\end{aligned}$$

□

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