STŘEDA FORMULA FOR CHARGE AND SPIN CURRENTS

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ABSTRACT. We consider a 2-dimensional Bloch–Landau–Pauli Hamiltonian for a spinful electron in a constant magnetic field subject to a periodic background potential. Assuming that the z-component of the spin operator is conserved, we compute the linear response of the associated spin density of states to a small change in the magnetic field, and identify it with the spin Hall conductivity. This response is in the form of a spin Chern marker, which is in general quantized to a half-integer, and to an integer under the further assumption of time-reversal symmetry. Our result is thus a generalization to the context of the quantum spin Hall effect to the well-known formula by Středa, which is formulated instead for charge transport.

CONTENTS

1. INTRODUCTION

The study of spin transport and the development of "spintronic" devices has recently attracted a lot of attention in the condensed matter community [31, 15, 34], which in turn initiated the mathematical analysis of spin transport [29, 30, 20, 22, 23]. A major part of the scientific activity in this direction has sparked after the discovery of time-reversal symmetric topological insulators, which can host the analogue of the quantum Hall effect but in the context of spin currents, namely the *quantum spin Hall effect* [16, 2, 14, 5].

The interest in the quantum Hall effect lies in the fact that a transport coefficient, namely the transverse charge conductivity σ_{12}, appears to be quantized (in appropriate physical units) up to an astounding precision: this was explained by relating this conductivity to a topological object, commonly known as the Chern number, which can only take integer values. One possible way to realize this connection was proposed by Středa in [35, 36], by equating σ_{12} to the variation with respect to an external magnetic field of the integrated density of states of the system, when the Fermi energy is assumed to stay in a spectral gap of the underlying Hamiltonian. Later, this and related results were proved in several contexts by different groups in the mathematical physics community: we refer to [9] for a recent account on this research line. For our discussion, it is nonetheless worth stressing that the Středa formula was proved by Cornean, Nenciu and Pedersen in [12] in the framework that we will adopt as well, namely that of gapped continuum Schrödinger operators in 2-dimensions modelling the dynamics of a spin-1/2 particle in a magnetic field subject to a $\mathbb{Z}^2$-periodic background potential.

Our goal is to modify and adapt the proof of the Středa formula provided by [12] to accommodate for a *conserved* spin degree of freedom. We will thus relate the spin Hall conductivity to the derivative with respect to the external magnetic field of the spin density of states, and obtain an expression for this derivative in terms of what we call a *spin Chern marker* (inspired by the topological markers in position space defined in [29, 21, 3, 6]). Our contribution can thus be seen as a formal proof of "spin Středa formulas" appearing in the physics literature [37, 27], and as a validation for the spin Chern number proposed by Prodan to investigate the quantum spin Hall topological phase [29], at least in a setting where the z-component of the spin operator is conserved.

The present paper fits in a broader research line focused on establishing the mathematical theory of spin trasport (see [20, 22, 23] and references therein). For example, some of the techniques from perturbation theory we employ have been used and generalized in the latter references to conduct a careful study of the linear response of a spin current to an external electric field, including the situation – which is not covered by the present work – of models which *do not* preserve the spin degree of freedom. To be more specific, it is worth mentioning that the definition of a spin current (and spin Hall conductivity) depends in general on the form of the quantum mechanical spin current operator. A conventional definition for the latter is $\mathbf{J}^z = -\frac{1}{2}\{\dot{\mathbf{X}}, S^z\}$, where $-\dot{\mathbf{X}} = -\mathrm{i}\,[H, \mathbf{X}]$ is the standard (charge) current operator associated to the Hamiltonian H for a particle with charge $q = -1$, while S^z denotes the z-component of the spin operator. On the basis of a "mesoscopic" continuity equation, it was proposed by Niu and collaborators in [32] that the "proper" definition should instead read $\mathbf{J}^z_{\mathrm{proper}} = -\mathrm{i}\,[H, \mathbf{X}S^z]$, which leads to well-posed spin currents also in the case of spin non-conserving Hamiltonians, but has the disadvantage of not being a translation-invariant operator. The use of this "proper" spin current operator requires setting up a new framework to study (spin) transport, and leads to more involved linear response formulas for the spin Hall conductivity [23]. The distinction between the two current operators has also led to a debate in the present context of the spin Středa formula: [37] adopts the "conventional" definition while [27] argues on the basis of the "proper" spin current operator. When H commutes with S^z, as we will assume, the two definitions coincide, and no ambiguity arises. We still consider the derivation of the spin Středa formula for spin non-preserving Hamiltonians an interesting research line, which we postpone to future work.

Although we formulate the results mainly for spin currents, if one substitutes the spin charge operator $-S^z$ with the electric charge operator $-\mathbf{1}$, our proofs go through unchanged, and our arguments (heavily inspired to [12]) can be used to cover charge currents and the quantum Hall setting as well. In particular, we obtain a partly new proof (presented with a slightly different strategy in [26]) of the quantization of the Hall conductivity as a multiple of an integer Chern number.

2. GENERALITIES ON BLOCH–LANDAU–PAULI HAMILTONIANS

Following [12], our reference Bloch–Landau–Pauli Hamiltonian acts on $L^2(\mathbb{R}^2) \otimes \mathbb{C}^2$ as (in appropriate units)

$$H_{B_1,B_2} := \frac{1}{2}\,\mathbf{P}(B_2)^2 + V(\mathbf{x}) \otimes \mathbf{1} + 2\,B_1\,\mathbf{1} \otimes s^z, \quad \mathbf{x} = (x_1, x_2) \in \mathbb{R}^2, \tag{1}$$

where

$$\mathbf{P}(B) := \left(-\mathrm{i}\nabla_{\mathbf{x}} - \frac{B}{2}\left(-x_2, x_1\right)\right) \otimes \mathbf{1} + \frac{1}{2}\left(-\partial_{x_2}V(\mathbf{x}), \partial_{x_1}V(\mathbf{x})\right) \otimes s^z$$

and $s^z := \sigma^z/2$ is the z-component of the spin operator (half of the third Pauli matrix). The magnetic momentum $\mathbf{P}(B)$ is modified to take into account the intrinsic spin-orbit coupling [19]. Physically, the parameters B_1 and B_2 are modelling the same magnetic field and should be equal, but for the sake of a more general discussion this is not needed for the moment; we will later simplify notation setting $B_1 = B_2 = B$ when appropriate. Observe in particular that

$$\left[P_j(B_2), S^z\right] = \left[H_{B_1,B_2}, S^z\right] = 0, \quad S^z := \mathbf{1} \otimes s^z, \quad j \in \{1, 2\}. \tag{2}$$

We assume V to be a smooth, real-valued, $\mathbb{Z}^2$-periodic potential. With this hypothesis, the Hamiltonian H_{B_1,B_2} is a selfadjoint operator bounded from below, and $C_0^\infty(\mathbb{R}^2) \otimes \mathbb{C}^2$ is a dense core. Moreover, we assume that H_{B_1,B_2} has a spectral gap around a certain (Fermi) energy E_F. We denote by Π_{B_1,B_2} the corresponding Fermi projection, defined by the following Riesz formula in terms of the resolvent of H_{B_1,B_2} [17]:

$$\Pi_{B_1,B_2} = \frac{\mathrm{i}}{2\pi}\oint_\Gamma \mathrm{d}w\left(H_{B_1,B_2} - w\mathbf{1}\right)^{-1}, \tag{3}$$

where Γ is a positively-oriented contour in the complex energy plane surrounding all the bands below E_F and contained in the resolvent set of H_{B_1,B_2}. Notice that the terms in the Hamiltonian which are proportional to S^z produce only bounded perturbations, therefore we can apply general results from the theory of magnetic Schrödinger operators [33, 11] and conclude that the resolvent operator has an integral kernel that decays away from the diagonal and has a logarithmic singularity on the diagonal [8, 4], that is,

$$\sup_{w \in \Gamma}\left\|\left(H_{B_1,B_2} - w\mathbf{1}\right)^{-1}(\mathbf{x}; \mathbf{y})\right\| \leq C_\Gamma\left(2 + \ln(1 + |\mathbf{x} - \mathbf{y}|^{-1})\right)\mathrm{e}^{-\beta_\Gamma|\mathbf{x} - \mathbf{y}|},$$

where C_Γ and β_Γ are positive constants that depend only on the contour Γ, and where the norm on the left-hand side is the matrix norm in $\mathbb{C}^2$. This implies that Π_{B_1,B_2} has a jointly continuous integral kernel with off-diagonal exponential decay, meaning that

$$\|\Pi_{B_1,B_2}(\mathbf{x}; \mathbf{y})\| \leq C\,\mathrm{e}^{-\alpha\,|\mathbf{x} - \mathbf{y}|},$$

for some positive constants $C, \alpha > 0$. Notice that the exponential decay is a consequence of Combes–Thomas estimates [7] combined with the existence of the spectral gap. The same is then true for the operators $[X_j, \Pi_{B_1,B_2}]$, $j \in \{1, 2\}$, where X_j denotes the position operator in the j-th direction: indeed

$$[X_j, \Pi_{B_1,B_2}](\mathbf{x}; \mathbf{y}) = (x_j - y_j)\,\Pi_{B_1,B_2}(\mathbf{x}; \mathbf{y})$$

as an identity between 2×2 matrices. In particular, the off-diagonal decay of the integral kernel of $[X_j, \Pi_{B_1,B_2}]$ implies via Schur's criterion that it is a bounded operator. Furthermore, all these operators are *magnetic covariant*, in the sense that their integral kernels satisfy

$$\mathrm{e}^{\mathrm{i}B_2\,(x_2\,n_1 - x_1 n_2)/2}K(\mathbf{x} - \mathbf{n}; \mathbf{y} - \mathbf{n})\mathrm{e}^{-\mathrm{i}B_2\,(y_2\,n_1 - yx_1 n_2)/2} = K(\mathbf{x}; \mathbf{y}) \quad \text{for all } \mathbf{n} \in \mathbb{Z}^2,$$

which is a crucial property in the computation of certain thermodynamic observables (cf. Section 3).

By *gauge-covariant magnetic perturbation theory* [10, 28, 11, 8, 9], the spectral gap around E_F persists also for neighbouring values of B_1 and B_2, and so we can consider Π_{B_1,B_2} as a function of B_1, B_2. In general, due to the singularity of the perturbation given by terms proportional to B_2, this will be very ill-behaved (not even continuous) if we look for example at the norm-topology of bounded operators on $L^2(\mathbb{R}^2) \otimes \mathbb{C}^2$, see for example [9, Corollary 1.2]. Nonetheless, there are certain other functions of Π_{B_1,B_2}, expressed in terms of its integral kernel, which are much more regular. For our purposes, the most relevant one is related to its *trace per unit volume*, defined for any magnetic covariant operator A with localized kernel as

$$\tau(A) := \frac{1}{|\Omega|}\int_\Omega \mathrm{d}\mathbf{x}\,\mathrm{Tr}_{\mathbb{C}^2}\left(A(\mathbf{x}; \mathbf{x})\right) = \frac{1}{|\Omega|}\int_\Omega \mathrm{d}\mathbf{x}\sum_{s \in \{\uparrow, \downarrow\}} A(\mathbf{x}, s; \mathbf{x}, s)$$

where $\Omega = (0,1)^2$ is the unit cell for the $\mathbb{Z}^2$-periodic potential. As a general remark, we will often use that this trace-like functional is *cyclic* on magnetic covariant operators with kernels that are exponentially localized away from the diagonal, namely that if A, B are such operators then $\tau(A\,B) = \tau(B\,A)$ (cf. [12, Eqn. (4.25)]).

Definition 2.1. The *integrated spin density of states* is defined as

$$\mathrm{IsDOS}(B_1, B_2) := \tau\left(S^z\,\Pi_{B_1,B_2}\right) = \frac{1}{2}\int_\Omega \mathrm{d}\mathbf{x}\,\left\{\Pi_{B_1,B_2}(\mathbf{x},\uparrow;\mathbf{x},\uparrow) - \Pi_{B_1,B_2}(\mathbf{x},\downarrow;\mathbf{x},\downarrow)\right\}.$$

Magnetic perturbation theory allows to show that $\mathrm{IsDOS}(B_1, B_2)$ is a smooth function of B_1, B_2: indeed, one can compute for example that (cf. [12, Eqn. (4.23)])

$$
\begin{aligned}
&\left.\frac{\partial}{\partial B_2}\,\mathrm{IsDOS}(B_1, B_2)\right|_{B_1=B_2=B} \\
&= -\frac{1}{4\pi}\tau\left(\int_\Gamma \mathrm{d}w\,S^z\,R_w(B)\,P_1(B)\,R_w(B)\,P_2(B)\,R_w(B) - \left(1 \leftrightarrow 2\right)\right)
\end{aligned}
\tag{4}
$$

where Γ is the usual complex-energy contour appearing in (3) and $R_w(B) := \left(H_{B_1=B,B_2=B} - w\mathbf{1}\right)^{-1}$. Note in particular that, to realize that the operators in the trace per unit volume have an exponentially localized integral kernel, one has to exploit the complex integral with respect to w [11].

Notice that only the perturbation due to the magnetic field B_2 is singular and has to be treated using gauge covariant magnetic perturbation theory, while the perturbation of the term proportional to B_1 is actually bounded and can be handled with the standard techniques of linear perturbation theory [17]. Therefore, for $\lambda := |\widetilde{B} - B_1|$ small enough, we have that

$$\left\|\Pi_{B_1,B_2} - \Pi_{\widetilde{B},B_2}\right\| \le \lambda C,$$

for some positive constant C. Hence, arguing e.g. as in [9, Lemma C.1], one can show that $\mathrm{IsDOS}(B_1, B_2) = \mathrm{IsDOS}(\widetilde{B}, B_2)$. We can conclude that the partial derivative of the $\mathrm{IsDOS}(B_1, B_2)$ with respect to B_2 evaluated in $B_1 = B_2 = B$ is actually equal to the total derivative of $\mathrm{IsDOS}(B,B) =: \mathrm{IsDOS}(B)$ with respect to B. Not to overburden the notation, we therefore set $B_1 = B_2 = B$ from here on out.

Remark 2.2. Using the fact that $\Pi_B := \Pi_{B,B}$ is a projector, so that in particular $\Pi_B^2 = \Pi_B$, (4) can be equivalently written as

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}B}\,\tau\left(S^z\,\Pi_B\right) &= \frac{\mathrm{d}}{\mathrm{d}B}\,\tau\left(S^z\,\Pi_B^2\right) \\
&= -\frac{1}{4\pi}\,\tau\Bigg(\int_\Gamma \mathrm{d}w\,S^z\,\Pi_B\,R_w(B)\,P_1(B)\,R_w(B)\,P_2(B)\,R_w(B) \\
&\qquad\qquad + S^z\,R_w(B)\,P_1(B)\,R_w(B)\,P_2(B)\,R_w(B)\,\Pi_B - \left(1 \leftrightarrow 2\right)\Bigg)
\end{aligned}
$$

Using cyclicity for the trace per unit volume and $[\Pi_B, S^z] = 0$ (in view of (2)), one can then manipulate the above and get

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}B}\,\mathrm{IsDOS}(B) \\
&= -\frac{1}{2\pi}\,\tau\left(\int_\Gamma \mathrm{d}w\,S^z\,\Pi_B\,R_w(B)\,P_1(B)\,R_w(B)\,P_2(B)\,R_w(B)\,\Pi_B - \left(1 \leftrightarrow 2\right)\right).
\end{aligned}
\tag{5}
$$

An analogous expression is used in [26] for the integrated density of states, obtained by replacing S^z with $\mathbf{1}$.

3. Spin Hall conductivity

Next we analyze the response of a $2d$ electron gas, whose one-particle description is modeled by the Hamiltonian $H_B := H_{B,B}$ defined in (1), to an (alternating) electric current. We will be interested in particular in the response of a transverse spin current and in computing the associated spin conductivity, adapting the strategy of [12]. As noted in the Introduction, when spin is not conserved the situation becomes more involved and this type of argument breaks down, thus requiring a new approach [23].

To compute the spin conductivity, we treat the electron gas as a grand canonical ensemble of non-interacting particles, initially (at time $t = -\infty$) in thermodynamic equilibrium. The gas is confined to a box $\Lambda_L := (-L, L]^2$ of linear size $L \geq 1$, with Dirichlet boundary conditions; we will later be interested in the thermodynamic limit $L \to \infty$. The restriction of the Hamiltonian H_B to the box with the specified boundary conditions is denoted as $H_B^{(L)}$. The asymptotic equilibrium state is modeled by the Fermi–Dirac distribution at temperature $T = \frac{1}{\beta}$ and at chemical potential μ in the non-interacting spectral gap:

$$\rho(-\infty) = f_{\mathrm{FD}}\big(H_B^{(L)}\big), \quad f_{\mathrm{FD}}(x) := \frac{1}{\mathrm{e}^{\beta(x-\mu)} + 1}, \quad x \in \mathbb{R}, \beta > 0, \mu \in \mathbb{R}. \tag{6}$$

The state then evolves adiabatically according to a time-dependent perturbed Hamiltonian

$$H_B^{(L)}(t) = H_B^{(L)} + V(t),$$

where the time-dependent electric potential is given by

$$V(\mathbf{x}, t) = \big(\mathrm{e}^{\mathrm{i}\omega t} + \mathrm{e}^{-\mathrm{i}\bar{\omega}t}\big) E x_2, \qquad t \leq 0, \, \mathbf{x} \in \Lambda_L, \, \Im\omega < 0, \, E \in \mathbb{R}.$$

Notice that the role of the time-adiabatic parameter is played by the imaginary part of ω.

The state of the system at $t \leq 0$ is described by a density matrix $\rho(t)$ that satisfies the Liouville equation

$$\mathrm{i}\partial_t\rho(t) = \left[H_B^{(L)}(t), \rho(t)\right], \quad \rho(-\infty) = f_{\mathrm{FD}}\big(H_B^{(L)}\big).$$

Using the Dyson expansion in the interaction picture one can argue that the solution to the Liouville equation is given by

$$\rho(0) = f_{\mathrm{FD}}\big(H_B^{(L)}\big) - \mathrm{i}\int_{-\infty}^{0}\mathrm{d}s\left[V^I(s), f_{\mathrm{FD}}\big(H_B^{(L)}\big)\right] + \mathcal{O}(E^2),$$

where $V^I(t) := \mathrm{e}^{\mathrm{i}tH_B^{(L)}}V(t)\mathrm{e}^{-\mathrm{i}tH_B^{(L)}}$. Assuming the validity of the linear response ansatz above, the spin current density that flows through the system at $t = 0$ is given by

$$\begin{aligned}
\mathbf{j}^{z,(L)} = {} & \frac{1}{|\Lambda_L|}\mathrm{Tr}_{\mathcal{H}_L}\left(f_{\mathrm{FD}}\big(H_B^{(L)}\big)\mathbf{J}_{\mathrm{proper}}^z\right) \\
& - \frac{\mathrm{i}}{|\Lambda_L|}\mathrm{Tr}_{\mathcal{H}_L}\left(\int_{-\infty}^{0}\mathrm{d}s\left[V^I(s), f_{\mathrm{FD}}\big(H_B^{(L)}\big)\right]\mathbf{J}_{\mathrm{proper}}^z\right) + \mathcal{O}(E^2).
\end{aligned} \tag{7}$$

The conductivity tensor is therefore given by the first order coefficient of the spin current density expansion in E, namely

$$j_\alpha^{z,(L)} = \left(\sigma_{\alpha,2}^{z,(L)}(\omega) + \sigma_{\alpha,2}^{z,(L)}(-\bar{\omega})\right)E, \qquad \alpha \in \{1, 2\}.$$

Since we are interested in the transverse conductivity, we consider only the first component of the spin current density, namely $j_1^{z,(L)}$. The equilibrium current, namely the first term in (7), vanishes, as $f_{\mathrm{FD}}\big(H_B^{(L)}\big)J_{1,\mathrm{proper}}^z = -\mathrm{i}\big[H_B^{(L)}, f_{\mathrm{FD}}\big(H_B^{(L)}\big)X_1 S^z\big]$ and the trace of a commutator is zero. Then, after integrating by parts and exploiting the cyclic properties of the trace, we get

$$\begin{aligned}
\sigma_{12}^{z,(L)}(B, T, \omega) = {} & \frac{\mathrm{i}}{\omega|\Lambda_L|}\mathrm{Tr}_{\mathcal{H}_L}\left(\left[X_2, f_{\mathrm{FD}}\big(H_B^{(L)}\big)\right]\left[H_B^{(L)}, X_1 S^z\right]\right) \\
& - \frac{\mathrm{i}}{\omega|\Lambda_L|}\mathrm{Tr}_{\mathcal{H}_L}\left(\int_{-\infty}^{0}\mathrm{d}s\,\mathrm{e}^{\mathrm{i}s\big(H_B^{(L)}+\omega\big)}P_2(B)\mathrm{e}^{-\mathrm{i}sH_B^{(L)}}\left[\left[H_B^{(L)}, X_1 S^z\right], f_{\mathrm{FD}}\big(H_B^{(L)}\big)\right]\right).
\end{aligned}$$

Since S^z is conserved, one can again use cyclicity of the trace to argue that the first term vanishes. In the second term, we can factor out the spin operator obtaining the so-called Kubo formula [18]

$$
\begin{aligned}
&\sigma_{12}^{z,(L)}(B,T,\omega) \\
&= -\frac{1}{\omega|\Lambda_L|}\mathrm{Tr}_{\mathcal{H}_L}\left(S^z\int_{-\infty}^{0}\mathrm{d}s\,\mathrm{e}^{\mathrm{i}s\left(H_B^{(L)}+\omega\right)}P_2(B)e^{-\mathrm{i}sH_B^{(L)}}\left[P_1(B),f_{\mathrm{FD}}\left(H_B^{(L)}\right)\right]\right).
\end{aligned}
$$

The previous formula can now be treated in the same way as in the charge current case, see [12, 11]. Due to the magnetic covariance of the operators in the trace, we first obtain that the spin conductivity admits a thermodynamic limit in the form of a trace per unit volume:

$$
\sigma_{12}^z(B,T,\omega) := \lim_{L\to\infty}\sigma_{12}^{z,(L)}(B,T,\omega).
$$

After that, we can perform the limit of zero temperature and zero frequency, where in particular the equilibrium state converges to the Fermi projection, obtaining a closed formula for the transverse spin conductivity which reads

$$
\begin{aligned}
\sigma_{12}^z(B) &:= \lim_{\omega\to0}\lim_{T\to0}\sigma_{12}^z(B,T,\omega) \\
&= -\frac{1}{4\pi}\tau\left(\int_{\Gamma}\mathrm{d}w\,S^z\,P_1(B)\,R_w(B)\,P_2(B)\,R_w^2(B) \,-\, S^z\,P_1(B)\,R_w^2(B)\,P_2(B)\,R_w(B)\right).
\end{aligned}
\tag{8}
$$

4. SPIN STŘEDA FORMULA

We are finally able to state our main result.

Theorem 4.1 (Spin Středa formula)**.** *For $\Pi_B := \Pi_{B,B}$*

$$
\sigma_{12}^z(B) = \frac{\mathrm{d}}{\mathrm{d}B}\,\mathrm{IsDOS}(B) = \frac{1}{2\pi}\,\mathrm{SCh}(\Pi_B),
\tag{9}
$$

where the spin Chern marker of Π_B is defined as

$$
\mathrm{SCh}(\Pi_B) := 2\pi\mathrm{i}\,\tau\big(S^z\,\Pi_B\,\big[[X_1,\Pi_B],[X_2,\Pi_B]\big]\,\Pi_B\big).
\tag{10}
$$

Proof. Since S^z commutes with $\mathbf{P}(B)$, the equality of the spin conductivity $\sigma_{12}^z(B)$ with the derivative of the integrated density of states is a simple consequence of the cyclicity for the trace per unit volume in the case of magnetic covariant operators with exponentially localized kernels, compare (4) and (8).

Instead, the proof of the second equality claimed in Theorem 4.1, which relates the integrated spin density of states with the spin Chern marker, relies on the following general result from perturbation theory (see e.g. [28]). To formulate its statement, recall that an operator A is called (*off-*)*diagonal* with respect to a projection $\Pi = \Pi^2$ whenever

$$
A = A^{\mathrm{D}} := \Pi\,A\,\Pi + \Pi^{\perp}\,A\,\Pi^{\perp} \quad (\text{resp. } A = A^{\mathrm{OD}} := \Pi\,A\,\Pi^{\perp} + \Pi^{\perp}\,A\,\Pi\,)
$$

with $\Pi^{\perp} := \mathbf{1} - \Pi$. It is clear that $A = A^{\mathrm{D}}$ if and only if $[A,\Pi] = 0$; therefore, every operator of the form $[A,\Pi] = [A^{\mathrm{OD}},\Pi]$ is off-diagonal.

Lemma 4.2. *Let A be an operator which is relatively bounded with respect to H_B. Define*

$$
\mathcal{I}(A) := \frac{\mathrm{i}}{2\pi}\oint_{\Gamma}\mathrm{d}w\,(H_B - w\mathbf{1})^{-1}\,A\,(H_B - w\mathbf{1})^{-1},
$$

where Γ is as in (3). Then $C := \mathcal{I}(A)$ solves

$$
\big[H_B, C\big] = \big[A, \Pi_B\big].
\tag{11}
$$

Moreover, $\mathcal{I}(A^{\mathrm{OD}}) = \mathcal{I}(A)^{\mathrm{OD}}$ is the unique solution of the above equation among operators which are off-diagonal with respect to the orthogonal decomposition of $L^2(\mathbb{R}^2)\otimes\mathbb{C}^2$ induced by Π_B.

Proof. Observe first of all that $\mathcal{I}(A)$ is a well-defined bounded operator, due to the relative boundedness of A and to the boundedness of the resolvent. Consider now the identity of bounded operators [1, Theorem 6.2.10] $R_w(B) [H_B, A] R_w(B) = [A, R_w(B)]$. Integrate both sides over Γ and multiply by $\mathrm{i}/2\pi$ to obtain

$$\left[H_B, \frac{\mathrm{i}}{2\pi} \oint_\Gamma \mathrm{d}w \, R_w(B) \, A \, R_w(B) \right] = \left[A, \frac{\mathrm{i}}{2\pi} \oint_\Gamma \mathrm{d}w \, R_w(B) \right] = [A, \Pi_B]$$

where the last equality is the Riesz formula (3) for the projection Π_B.

Since $[A, \Pi_B] = [A^{\mathrm{OD}}, \Pi_B]$, $\mathcal{I}(A^{\mathrm{OD}})$ solves (11), and moreover it is off-diagonal as the resolvent is a diagonal operator (it commutes with H_B and therefore with its spectral projection Π_B), which implies that $\mathcal{I}(A^{\mathrm{OD}}) = \mathcal{I}(A)^{\mathrm{OD}}$. If now C is another off-diagonal solution to (11), then $\mathcal{I}(A^{\mathrm{OD}}) - C$ commutes with H_B and is therefore both diagonal and off-diagonal. We conclude that $\mathcal{I}(A^{\mathrm{OD}}) - C = 0$, which proves the uniqueness of $\mathcal{I}(A^{\mathrm{OD}})$ among off-diagonal solutions to (11). $\qquad\square$

Let us use the above Lemma to compute $\big[[\Pi_B, A_1], [\Pi_B, A_2]\big]$ assuming that A_1 and A_2 are bounded off-diagonal operators with respect to Π_B. Dropping the subscript B, we have

$$[[\Pi, A_1], [\Pi, A_2]] = \left[\left[H, \frac{\mathrm{i}}{2\pi} \oint_\Gamma \mathrm{d}w \, R_w A_1 R_w \right], \left[H, \frac{\mathrm{i}}{2\pi} \oint_{\Gamma'} \mathrm{d}w' \, R_{w'} A_2 R_{w'} \right] \right]$$

$$= \left(\frac{\mathrm{i}}{2\pi} \right)^2 \oint_\Gamma \mathrm{d}w \oint_{\Gamma'} \mathrm{d}w' \left\{ R_w [H, A_1] R_w R_{w'} [H, A_2] R_{w'} - R_{w'} [H, A_2] R_{w'} R_w [H, A_1] R_w \right\}.$$

We have chosen the contours Γ, Γ' so that both surround the relevant spectral island of H and Γ' has a slightly smaller diameter than Γ. For future reference, let us denote by $D \subset \mathbb{C}$ the region surrounded by Γ, and by $D' \subset D$ the region surrounded by Γ'.

We further elaborate the above expression by using the resolvent identity $R_w R_{w'} = (w - w')^{-1} (R_w - R_{w'})$. We conclude that $\big[[\Pi, A_1], [\Pi, A_2]\big] = \mathrm{I} + \mathrm{II} + \mathrm{III} + \mathrm{IV}$ with

$$\mathrm{I} := \left(\frac{\mathrm{i}}{2\pi} \right)^2 \oint_\Gamma \mathrm{d}w \oint_{\Gamma'} \mathrm{d}w' \, \frac{1}{w - w'} R_w [H, A_1] R_w [H, A_2] R_{w'},$$

$$\mathrm{II} := -\left(\frac{\mathrm{i}}{2\pi} \right)^2 \oint_\Gamma \mathrm{d}w \oint_{\Gamma'} \mathrm{d}w' \, \frac{1}{w - w'} R_w [H, A_1] R_{w'} [H, A_2] R_{w'},$$

$$\mathrm{III} := -\left(\frac{\mathrm{i}}{2\pi} \right)^2 \oint_\Gamma \mathrm{d}w \oint_{\Gamma'} \mathrm{d}w' \, \frac{1}{w' - w} R_{w'} [H, A_2] R_{w'} [H, A_1] R_w,$$

$$\mathrm{IV} := \left(\frac{\mathrm{i}}{2\pi} \right)^2 \oint_\Gamma \mathrm{d}w \oint_{\Gamma'} \mathrm{d}w' \, \frac{1}{w' - w} R_{w'} [H, A_2] R_w [H, A_1] R_w.$$

Let us show how to compute the term I. We rewrite

$$\mathrm{I} = \frac{\mathrm{i}}{2\pi} \oint_\Gamma \mathrm{d}w \, R_w [H, A_1] R_w [H, A_2] \left(\frac{\mathrm{i}}{2\pi} \oint_{\Gamma'} \mathrm{d}w' \, \frac{R_{w'}}{w - w'} \right).$$

We multiply the integrand in parenthesis by $\mathbf{1} = \Pi + \Pi^\perp$. Using that R_w is a diagonal operator we can write

$$\frac{\mathrm{i}}{2\pi} \oint_{\Gamma'} \mathrm{d}w' \, \frac{R_{w'}}{w - w'} = \frac{\mathrm{i}}{2\pi} \oint_{\Gamma'} \mathrm{d}w' \, \frac{\Pi R_{w'} \Pi}{w - w'} + \frac{\mathrm{i}}{2\pi} \oint_{\Gamma'} \mathrm{d}w' \, \frac{\Pi^\perp R_{w'} \Pi^\perp}{w - w'}.$$

Let us look at the second term on the right-hand side of the above equality. Since $w \notin D'$, the function $w' \mapsto \Pi^\perp R_{w'} \Pi^\perp / (w - w')$ is *holomorphic* in the region D': indeed, the singularity of the resolvent at real energies w' in the spectral island below the gap is removed by the presence of the projection $\Pi^\perp$ away from this spectral subspace. We conclude that its integral over Γ' vanishes by Cauchy's theorem. As for the first integral, instead, we observe that the function $w' \mapsto \Pi R_{w'} \Pi$ is holomorphic in the *exterior* region $\mathbb{C} \setminus \overline{D'}$: this time the projection Π removes the singularities

of the resolvent above the spectral gap. Using Cauchy's integral formula for unbounded domains [24, Problem 14.14], we conclude that

$$\frac{\mathrm{i}}{2\pi} \oint_{\Gamma'} \mathrm{d}w' \, \frac{\Pi \, R_{w'} \, \Pi}{w - w'} = \frac{1}{2\pi\mathrm{i}} \oint_{\Gamma'} \mathrm{d}w' \, \frac{\Pi \, R_{w'} \, \Pi}{w' - w} = \Pi \, R_{\infty} \, \Pi - \Pi \, R_w \, \Pi = -\Pi \, R_w \, \Pi,$$

where $\Pi \, R_{\infty} \, \Pi := \lim_{|z| \to \infty} \Pi \, R_z \, \Pi = 0$ since $\left\| \Pi \, R_w \, \Pi \right\| = 1/\mathrm{dist}(z, \sigma(\Pi \, H \, \Pi))$. Finally

$$\mathrm{I} = -\frac{\mathrm{i}}{2\pi} \oint_{\Gamma} \mathrm{d}w \, R_w \, [H, A_1] \, R_w \, [H, A_2] \, R_w \, \Pi.$$

The other three terms, namely $\mathrm{II}, \mathrm{III}$ and IV, can be computed using the same strategy; moreover, we can freely change the integration contour from Γ' to Γ in the final expressions due to the analyticity of the resolvent operator in the spectral parameter. We conclude that $-\mathrm{i}\left[[\Pi, A_1], [\Pi, A_2] \right] = \left(\Pi \, T_{A_1, A_2} \, \Pi - \Pi^{\perp} \, T_{A_1, A_2} \, \Pi^{\perp} \right)$ where

$$T_{A_1, A_2} := \oint_{\Gamma} \mathrm{d}w \left\{ R_w \left(\mathrm{i}[H, A_1] \right) R_w \left(\mathrm{i}[H, A_2] \right) R_w - R_w \left(\mathrm{i}[H, A_2] \right) R_w \left(\mathrm{i}[H, A_1] \right) R_w \right\} \qquad (12)$$

with $R_w = R_w(B)$. In particular $\Pi \, T_{A_1, A_2} \, \Pi = -\mathrm{i} \, \Pi \left[[\Pi, A_1], [\Pi, A_2] \right] \Pi$.

We apply now the above considerations to the operators $A_j = [X_j, \Pi_B]$, $j \in \{1, 2\}$, which are indeed bounded and off-diagonal with respect to $\Pi = \Pi_B$. Notice first of all that, by the Jacobi identity and the fact that $\dot{\mathbf{X}} = \mathbf{P}$,

$$\mathrm{i}\left[H_B, [X_j, \Pi_B] \right] = -\mathrm{i}\left[\Pi_B, [H_B, X_j] \right] = -\left[\Pi_B, P_j(B) \right]$$

if all terms are sandwiched between $R_w(B)$. Plugging the above into (12) and performing some simple algebra, we conclude that

$$\mathrm{i} \, \Pi \left[[X_1, \Pi], [X_2, \Pi] \right] \Pi = \Pi \, T_{[X_1, \Pi], \, [X_2, \Pi]} \, \Pi$$

$$= -\frac{1}{2\pi} \oint_{\Gamma} \mathrm{d}w \left\{ \Pi \, R_w \, P_1 \, R_w \, P_2 \, R_w \, \Pi - (1 \leftrightarrow 2) \right\}$$

$$+ \frac{1}{2\pi} \oint_{\Gamma} \mathrm{d}w \left\{ \Pi \, R_w \, \Pi \, P_1 \, \Pi \, R_w \, \Pi \, P_2 \, \Pi \, R_w \, \Pi - (1 \leftrightarrow 2) \right\}.$$

We now multiply the above operator identity by S^z on the left and take the trace per unit volume. Observe that S^z commutes with all the operators appearing on the third line of the above in view of (2); the cyclicity property then implies that this line does not contribute to the trace per unit volume, being skew-symmetric in the exchange of the indices $(1 \leftrightarrow 2)$. Therefore by comparing the result equation to (5) and (10), we see that this is exactly the claimed second equality in (9). This concludes the proof of Theorem 4.1.   □

5. Quantization of the spin Hall conductivity

The spin Středa formula (9) can be used to deduce that the spin Hall conductivity σ_{12}^z is *quantized* to a half-integer or integer in units of $1/2\pi$. Indeed, under the assumption (2) the Fermi projection splits as a direct sum of two projections, one corresponding to spin "up" and one corresponding to spin "down":

$$\Pi_B = \Pi_B^{\uparrow} \oplus \Pi_B^{\downarrow}, \quad \Pi_B^{\uparrow/\downarrow} := P^{\uparrow/\downarrow} \Pi_B \, P^{\uparrow/\downarrow}, \quad P^{\uparrow/\downarrow} := \frac{1}{2} \mathbf{1} \otimes (\mathbf{1} \pm \sigma^z).$$

It is not difficult to see that then

$$\mathrm{SCh}(\Pi_B) = \frac{1}{2} \left(\mathrm{Ch}\big(\Pi_B^{\uparrow}\big) - \mathrm{Ch}\big(\Pi_B^{\downarrow}\big) \right), \text{ where } \mathrm{Ch}(\Pi) := 2\pi\mathrm{i} \, \tau \left(\Pi \left[[X_1, \Pi], [X_2, \Pi] \right] \Pi \right).$$

$\mathrm{Ch}(\Pi)$ is the *Chern marker* (sometimes called also *Chern character*) of the projection Π. It can be argued (see e.g. [9]) that $\mathrm{Ch}(\Pi_B)$ is a *continuous* function of B (as long as the spectral gap around the Fermi energy does not close), which attains *integer values*: therefore $\mathrm{Ch}\big(\Pi_B^{\uparrow/\downarrow}\big)$ must be both *constant integers* in B if the spectral gap remains open, and we deduce that $\mathrm{SCh}(\Pi_B) \in \frac{1}{2}\mathbb{Z}$.

Notice that when $B_1 = B_2 = 0$, then $H_{0,0}$ commutes with the fermionic time-reversal operator $\Theta := \mathrm{i}(\mathbf{1} \otimes \sigma^y)K$, where K is the complex conjugation operator on $L^2(\mathbb{R}^2) \otimes \mathbb{C}^2$. This implies

in particular that $\mathrm{Ch}\big(\Pi_0^\downarrow\big) = \mathrm{Ch}\big(\Theta\,\Pi_0^\uparrow\,\Theta^{-1}\big) = -\mathrm{Ch}\big(\Pi_0^\uparrow\big)$, cf. [25]. We therefore conclude that actually

$$\mathrm{SCh}(\Pi_0) = \mathrm{Ch}\big(\Pi_0^\uparrow\big) \in \mathbb{Z}.$$

The parity of this integer is the *spin Chern number* proposed in [29] as a $\mathbb{Z}_2$-valued topological invariant to classify (disordered) time-reversal symmetric topological insulators. In the setting of discrete Bogoliubov–de Gennes Hamiltonians and with the assumption of conserved spin, the equality between the spin conductivity and the spin Chern number has been proved in [13]. A study of the spin Chern number in relation to spin transport and its robustness to small perturbations that break spin conservation can be found in [29, 30], see also the discussion in [23].

REFERENCES

[1] W. O. Amrein, A. Boutet de Monvel, and V. Georgescu. C_0-*groups, commutator methods and spectral theory of N-body Hamiltonians*. No. 135 in Progress in Mathematics (Birkhäuser Verlag, Basel, 1996).

[2] B. A. Bernevig, T. L. Hughes, and S.-C. Zhang. Quantum Spin Hall Effect and Topological Phase Transition in HgTe Quantum Wells. *Science* **314** (2006), 1757–1761.

[3] R. Bianco and R. Resta: Mapping topological order in coordinate space. Phys. Rev. B **84** (2011), 241106.

[4] K. Broderix, D. Hundertmark, and H. Leschke. Continuity properties of Schrödinger semigroups with magnetic fields. *Rev. Math. Phys.* **12** (2000), 181-225.

[5] C. Brüne, A. Roth, E. G. Novik, M. König, H. Buhmann, E. M. Hankiewicz, W. Hanke, J. Sinova, and L. W. Molenkamp. Evidence for the ballistic intrinsic spin Hall effect in HgTe nanostructures. *Nat. Phys.* **6** (2010), 448–454.

[6] M. D. Caio, G. Möller, N. R. Cooper and M. J. Bhaseen: Topological marker currents in Chern insulators. *Nat. Phys.* **15** (2019), 257–261 .

[7] J. M. Combes and L. Thomas. Asymptotic behavior of eigenfunctions for multiparticle Schrödinger operators. *Commun. Math. Phys.* **34** (1973), 251–270.

[8] H. D. Cornean. On the Lipschitz continuity of spectral bands of Harper-like and magnetic Schrödinger operators. *Ann. Henri Poincaré* **11** (2010), 973—990.

[9] H. D. Cornean, D. Monaco, and M. Moscolari. Beyond Diophantine Wannier diagrams: Gap labelling for Bloch-Landau Hamiltonians. To appear in *J. Eur. Math. Soc.* Preprint available online at `arXiv:1810.05623` (2018).

[10] H. D. Cornean and G. Nenciu. On eigenfunction decay of two dimensional magnetic Schrödinger operators. *Commun. Math. Phys.* **192** (1998), 671–685.

[11] H. D. Cornean and G. Nenciu. The Faraday effect revisited: Thermodynamic limit. *J. Funct. Anal.* **257** (2009), 2024–2066.

[12] H. D. Cornean, G. Nenciu, and T. Pedersen. The Faraday effect revisited: General theory. *J. Math. Phys.* **47** (2006), 013511.

[13] G. De Nittis and H. Schulz-Baldes. The non-commutative topology of two-dimensional dirty superconductors. *J. Geometry Phys.*, **124** (2018), 100–123.

[14] M. Z. Hasan and C. L. Kane. Colloquium: Topological insulators. *Rev. Mod. Phys.* **82** (2010), 3045–3067.

[15] T. Jungwirth, J. Wunderlich, and K. Olejník. Spin Hall effect devices. *Nat. Mater.* **11** (2012), 382–390.

[16] C. L. Kane and E. J. Mele. Z_2 Topological Order and the Quantum Spin Hall Effect. *Phys. Rev. Lett.* **95** (2005), 146802.

[17] T. Kato. *Perturbation theory for linear operators* (Springer, Berlin, 1966).

[18] R. Kubo. Statistical-mechanical theory of irreversible processes I: General theory and simple applications to magnetic and conduction problems. *J. Phys. Soc. Jpn.* **12** (1957), 570–586.

[19] J. M. Luttinger and W. Kohn. Motion of Electrons and Holes in Perturbed Periodic Fields. *Phys. Rev.* **97** (1955), 869–883.

[20] G. Marcelli. *A mathematical analysis of spin and charge transport in topological insulators*. PhD Thesis, "La Sapienza" Università di Roma (2018).

[21] G. Marcelli, D. Monaco, M. Moscolari and G. Panati: The Haldane model and its localization dichotomy. *Rend. Mat. Appl.* **39**(2) (2018), 307–327. Extended version available online at `arXiv:1909.03298`.

[22] G. Marcelli, G. Panati, and C. Tauber. Spin conductance and spin conductivity in topological insulators: Analysis of Kubo-like terms. *Ann. Henri Poincaré* **20** (2019), 2071–2099.

[23] G. Marcelli, G. Panati, and S. Teufel. A new approach to transport coefficients in the quantum spin Hall effect. Preprint available online at `arXiv:2004.00956` (2020).

[24] A. I. Markushevich. *Theory of Functions of a Complex Variable, Volume 1* (Prentice-Hall, New Jersey, 1965).

[25] D. Monaco and G. Panati. Symmetry and localization in periodic crystals: triviality of Bloch bundles with a fermionic time-reversal symmetry. *Acta App. Math.* **137** (2015), 185–203.

[26] M. Moscolari. *On the localization dichotomy for gapped quantum systems*. PhD Thesis, "La Sapienza" Università di Roma (2019).

[27] S. Murakami. Quantum Spin Hall Effect and Enhanced Magnetic Response by Spin-Orbit Coupling. *Phys. Rev. Lett.* **97** (2006), 236805.
[28] G. Nenciu. On asymptotic perturbation theory for quantum mechanics. Almost invariant subspaces and gauge invariant magnetic perturbation theory. *J. Math. Phys.* **43** (2002), 1273.
[29] E. Prodan. Robustness of the spin-Chern number. *Phys. Rev. B* **80** (2009), 125327.
[30] H. Schulz-Baldes. Persistence of Spin Edge Currents in Disordered Quantum Spin Hall Systems. *Commun. Math. Phys.*, **324** (2013), 589–600.
[31] J. Schliemann. Spin Hall Effect. *Int. J. Mod. Phys. B* **20** (2006), 1015–1036.
[32] J. Shi, P. Zhang, D. Xiao, and Q. Niu. Proper Definition of Spin Current in Spin-Orbit Coupled Systems. *Phys. Rev. Lett.* **96** (2006), 076604.
[33] B. Simon. Schrödinger semigroups. *Bull. Amer. Math. Soc. (N.S.)* **3** (1982), 447–526.
[34] J. Sinova, S. O. Valenzuela, J. Wunderlich, C. H. Back, and T. Jungwirth. Spin Hall effects. *Rev. Mod. Phys.* **87** (2015), 1213–1260.
[35] P. Středa. Theory of quantised Hall conductivity in two dimensions. *J. Phys. C: Solid State Phys.* **15** (1982), L717–L721.
[36] P. Středa. Quantised Hall effect in a two-dimensional periodic potential. *J. Phys. C: Solid State Phys.* **15** (1982), L1299–L1303.
[37] M.-F. Yang and M.-C. Chang. Středa-like formula in the spin Hall effect. *Phys. Rev. B* **73** (2006), 073304.

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