Quantum (spin) Hall conductivity: Kubo-like formula (and beyond)

Giovanna Marcelli
joint works with D. Monaco (*Roma Tre*, Roma), G. Panati (*La Sapienza*, Roma), C. Tauber (*ETH*, Zürich) and S. Teufel (Universität Tübingen)

[MMPTe]: in progress and [MPTa]: arXiv:1801.02611

EBERHARD KARLS UNIVERSITÄT TÜBINGEN

Recent Progress in Mathematics of Topological Insulators
4th September, 2018

Seminar outline

Experimental setups for QHE and QSHE

Linear response coefficients: σ_{ij} for both QHE and QSHE

A model for quantum transport

- Charge and spin current operator
- Construction of the NEASS
- Adiabatic conductivity $\sigma_{ij}^{\varepsilon}$: Kubo-like formula and beyond

Spin conductance and spin conductivity: analysis of Kubo-like terms

Experimental setup (schematic):

1. Quantum Hall charge effect
2. Quantum Hall spin effect

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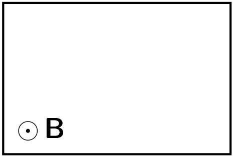

B: external magnetic field

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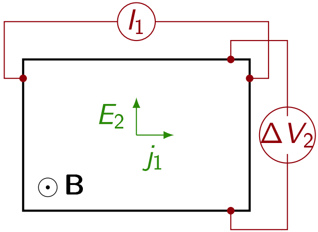

Conductance $G_{12} := -\frac{I_1}{\Delta V_2}$

Conductivity $\sigma_{12} := \frac{j_1}{E_2}$

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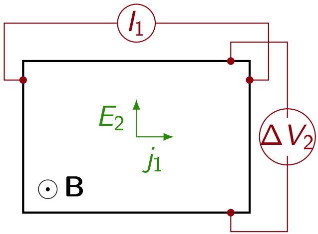

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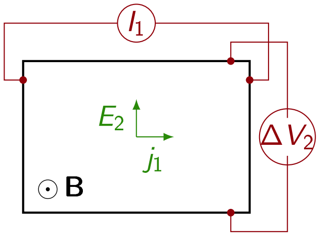

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$$\boxed{G_{12} \simeq n\frac{e^2}{h}, \quad n \in \mathbb{Z}}$$

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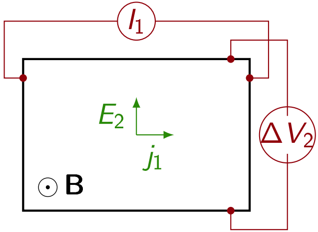

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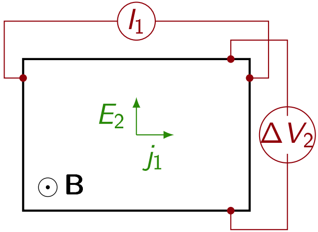

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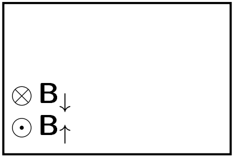

$\mathbf{B}_\uparrow$, $\mathbf{B}_\downarrow$: from spin-orbit coupling

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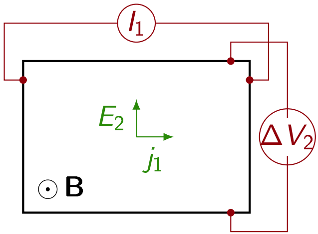

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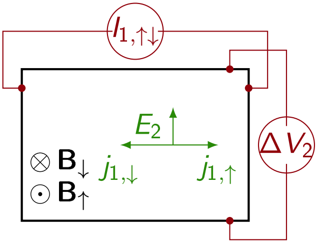

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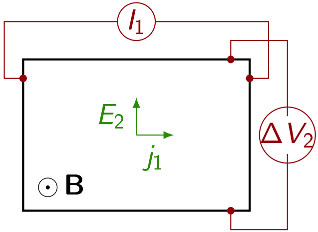

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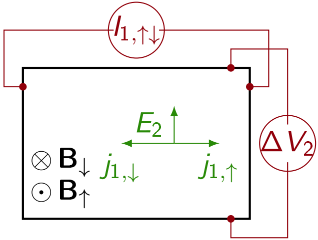

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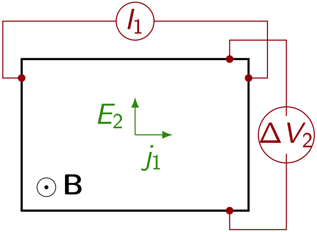

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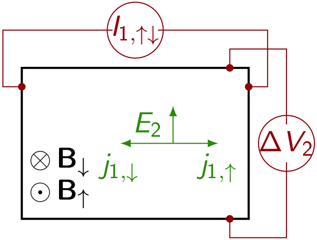

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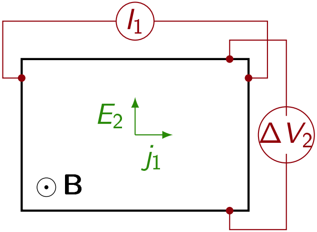

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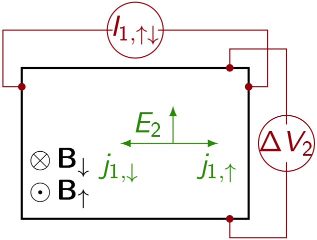

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$$\boxed{\sigma_{12}^{s_z} \overset{?}{=} G_{12}^{s_z} \overset{?}{\in} \frac{e}{2\pi}\mathbb{Z}}$$

Linear response coefficients: σ_{ij}

We are going to

- study the linear response coefficients of a gapped, periodic and one-particle quantum system to the perturbation of a small electric field, modeled by a potential $-\varepsilon X_j$ with $\varepsilon \ll 1$, in terms of the conductivity σ_{ij}
  - for both charge (Quantum Hall effect) and spin (Quantum spin Hall effect) transport.
- derive formulas via an argument which is as model-independent as possible via the method of non-equilibrium almost-stationary state (NEASS)
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A model for quantum transport

Assumption (H) on the unperturbed model

- $\mathcal{H} := L^2(\mathcal{X}) \otimes \mathbb{C}^N$,
  $\mathcal{X} = \mathbb{R}^d$ or $\mathcal{X} =$ discrete d-dimensional crystal $\subset \mathbb{R}^d$.
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- H_0 is a periodic gapped operator on $\mathcal{H}$ and bounded from below
  - Bravais lattice of translations $= \Gamma \simeq \mathbb{Z}^d$

$$[H_0, T_\gamma] = 0 \quad \forall \gamma \in \Gamma.$$

  - via Bloch–Floquet representation $H_0 \simeq \int_{\mathbb{T}^d}^{\oplus} \mathrm{d}k \, H_0(k)$,
    $H_0(k)$ acts on $\mathcal{H}_\mathrm{f} := L^2(\mathcal{C}_1) \otimes \mathbb{C}^N$, $\mathcal{C}_1 \simeq \mathbb{R}^d / \Gamma$.

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  - $$H_0 : \mathbb{R}^d \to \mathcal{L}(\mathcal{D}_\mathrm{f}, \mathcal{H}_\mathrm{f}), \quad k \mapsto H_0(k)$$
    is a smooth equivariant map taking values in the self-adjoint operators with dense domain $\mathcal{D}_\mathrm{f} \subset \mathcal{H}_\mathrm{f}$. $\mathcal{L}(\mathcal{D}_\mathrm{f}, \mathcal{H}_\mathrm{f})$ is the space of bounded operators from $\mathcal{D}_\mathrm{f}$, equipped with the graph norm of $H_0(0)$, to $\mathcal{H}_\mathrm{f}$.

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Remark The above assumptions are satisfied

- in most tight-binding models (discrete case)

- by gapped, periodic Schrödinger operators

$$H_0 = \frac{1}{2}(-\mathrm{i}\nabla - A(x))^2 + V(x)$$

  under standard hypotheses of relative boundedness of the potentials w.r.t. $-\Delta$ (continuum case).

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Definition Let $\mathcal{H}_1, \mathcal{H}_2 \in \{\mathcal{D}_\mathrm{f}\,, \mathcal{H}_\mathrm{f}\}$

$\mathcal{P}(\mathcal{H}_1, \mathcal{H}_2) := \{$ Γ-periodic A with smooth fibration $\mathbb{R}^d \to \mathcal{L}(\mathcal{H}_1, \mathcal{H}_2)$ $\}$

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Perturbed model

Add an electric field in direction j of small intensity $\varepsilon \in [0,1]$:

$$H^{\varepsilon} := H_0 - \varepsilon X_j$$

Current operator

$S = \mathrm{Id}_{L^2(\mathcal{X})} \otimes s$ self-adjoint, acting only on $\mathbb{C}^N$ (internal degrees of freedom)

- $s = \mathrm{Id} \longrightarrow$ charge current (QHE)
- $s = s_z = \sigma_z/2 \longrightarrow$ spin current (QSHE) proposed by [SZXN '06]

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$\vec{J}$ versus periodicity

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$\vec{J}$ is not periodic

$$\vec{J} = \mathrm{i}[H_0, S\vec{X}]$$

if and only if $[H_0, S] \neq 0$ (for $S = \mathrm{Id}_{L^2(\mathcal{X})} \otimes s_z$ in the Kane–Mele model: $\lambda_{Rashba} \neq 0$).

Simple but new observation in [M., Panati, Tauber '18]:

$$T_{\vec{\gamma}} \vec{J} T_{\vec{\gamma}}^{-1} = \vec{J} - \vec{\gamma}\,\mathrm{i}[H_0, S] \qquad \forall \vec{\gamma} \in \Gamma.$$

$\rightsquigarrow$ the periodicity is restored on mesoscopic scale!

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Trace per unit volume

$$\tau(A) := \lim_{\substack{L\to\infty \\ L\in 2\mathbb{N}+1}} \frac{1}{|\mathcal{C}_L|}\operatorname{Tr}(\chi_L A \chi_L), \quad |\mathcal{C}_L| = L^d\,|\mathcal{C}_1|$$

Lemma 1.
Let A be periodic and $\chi_K A \chi_K \in \mathcal{B}_1(\mathcal{H})$ $\forall$ compact set K. Then $\tau(A)$ is well-defined and

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$$\tau(A) := \lim_{\substack{L\to\infty \\ L\in 2\mathbb{N}+1}} \frac{1}{|\mathcal{C}_L|} \mathrm{Tr}(\chi_L A \chi_L), \quad |\mathcal{C}_L| = L^d \, |\mathcal{C}_1|$$

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Let A be periodic and $\chi_K A \chi_K \in \mathcal{B}_1(\mathcal{H})$ $\forall$ compact set K. Then $\tau(A)$ is well-defined and

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Perturbed model

Add an electric field in direction j of small intensity $\varepsilon \in [0,1]$:

$$H^{\varepsilon} := H_0 - \varepsilon X_j$$

Theorem 3 (M., Monaco, Panati, Teufel '18).

One can construct a non-equilibrium almost-stationary state (NEASS) Π^{ε} for H^{ε} such that H_0 enjoys Assumption (H):

1. $\Pi^{\varepsilon} = e^{-i\varepsilon S}\Pi_0 e^{i\varepsilon S}$ *for some bounded, periodic and self-adjoint operator S;*

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Proof.

- $\mathcal{I}(\,\cdot\,)$ = inverse Liouvillian: for $A = A^{\mathrm{OD}} := \Pi_0 A \Pi_0^{\perp} + \Pi_0^{\perp} A \Pi_0 \in \mathcal{P}(\mathcal{H}_{\mathrm{f}})$

$$\mathcal{I}(A) := \frac{\mathrm{i}}{2\pi} \oint_C \mathrm{d}z\, (H_0 - z\mathrm{Id})^{-1} \, [A, \Pi_0] \, (H_0 - z\mathrm{Id})^{-1} \in \mathcal{P}(\mathcal{H}_{\mathrm{f}}, \mathcal{D}_{\mathrm{f}})$$

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Remark: Justification for using the NEASS (in progress)

Consider the time-dependent Hamiltonian

$$H^{\varepsilon}_{\mathrm{switch}}(t) := H_0 - f(t)\,\varepsilon\, X_j,$$

where $f : \mathbb{R} \to [0,1]$ is a smooth function : $f(t) = 0$ for all $t \leq 0$ and $f(t) = 1$ for all $t \geq T > 0$.

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Then

$\|\rho^{\varepsilon}(t) - \Pi^{\varepsilon}\| = \mathcal{O}(\varepsilon^2)$ uniformly on bounded intervals in time.

This statement is already proved in the context of interacting models on lattices [Teufel, '17].

NEASS bypasses the LRA and the justification of its validity, and it is independent of the shape of the switching function!

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Response currents

We want to compute the response of a current to the perturbation of a weak electric field, in the regime of linear approximation $\rightsquigarrow$ in terms of the adiabatic conductivity tensor $\sigma^{\varepsilon}_{ij}$

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$[H_0, S] \neq 0$: beyond-Kubo-like formula

Theorem 4 (M., Monaco, Panati, Teufel '18).

1. *Let H_0 satisfy Assumption (H) and let $H^\varepsilon = H_0 - \varepsilon X_j$.*
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---

[1] If H_0 enjoys spatial symmetries hypothesis 2 is satisfied (*e. g.* the Kane–Mele model is invariant under $2\pi/3$ rotation).

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Remark *conditional* cyclicity of $\tau(\,\cdot\,) \implies$ persistent current vanishes automatically and the beyond-Kubo-like terms vanish. In $d = 2$ the Kubo-term is equal to the (Spin) Chern number for ($S = \mathrm{Id} \otimes s_z$) $S = \mathrm{Id}$ (whenever H_0 is time-reversal symmetric).

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Remark For $S = \mathrm{Id}$ this result agrees with [AG '98, BES '94, BGKS '05, AW '15 ...] and for $S = \mathrm{Id} \otimes s_z$ it agrees with [Pr '09, Sch '13].

Inspired by the Kubo theory of charge transport [ASS, '94]

- we define the Kubo-like spin conductance $G_K^{s_z}$ and prove that
- for any gapped, periodic, one-particle and near-sighted discrete Hamiltonian $G_K^{s_z}$ is well-defined
- the equality

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Kubo-like spin conductance and conductivity: mathematical setting

- Hilbert space $\mathcal{H}_{\text{disc}} := \ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^N \otimes \mathbb{C}^2$

  For $A \in \mathcal{B}(\mathcal{H}_{\text{disc}})$
  $A_{\mathbf{m},\mathbf{n}} := \left\langle \delta_{\mathbf{m}}^{(k)}, A\, \delta_{\mathbf{n}}^{(k)} \right\rangle_{\{k \in \{1,\dots,2N\}\}} \in \mathrm{End}_{2N}(\mathbb{C})$

- Hamiltonian H_0 is bounded, self-adjoint
  1. periodic: $H_{0\,\mathbf{m},\mathbf{n}} = H_{0\,\mathbf{m}-\mathbf{p},\mathbf{n}-\mathbf{p}}\ \forall\, \mathbf{m},\mathbf{n},\mathbf{p} \in \mathbb{Z}^2$
  2. near-sighted
  3. admits a spectral gap

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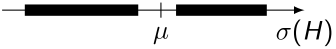

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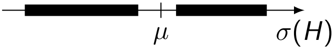

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Conclusion

1. We have analyzed quantum transport of charge and spin via space-adiabatic perturbation theory (NEASS) avoiding the LRA.
2. We have established a Kubo-like formula for the adiabatic conductivity related to the current operator $\vec{J} = \mathrm{i}[H_0, S\vec{X}]$ with corrections when S is not conserved.
3. In charge- or spin-preserving models, we have established quantization of conductivities via (spin) Chern numbers.
4. Even if $[H_0, s_z] \neq 0$, then Kubo-like spin conductivity and spin conductance are well-defined and coincide using the "proper" spin current $\vec{J}$, due to $\tau(\mathcal{T}_z) = 0$, because periodicity and spin conservation are restored on average.

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Perspectives

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2. Define and analyze of the beyond-Kubo-like terms in terms of conductance $\rightsquigarrow$ does the equality $G_{ij}^{s_z} = \sigma_{ij}^{s_z}$ still hold?

3. Study higher-order corrections in ε to the formula for the adiabatic conductivity σ_{ij}.

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