A new approach to transport coefficients in the quantum spin Hall effect and to purely linear response of the quantum Hall current

Giovanna Marcelli

joint works with D. Monaco, G. Panati (*La Sapienza*, Roma) and S. Teufel (*Universität Tübingen*)

Ann. Henri Poincaré (2021), arXiv:2112.03071

SISSA

Quantum before Christmas - Milano, 21/12/2021

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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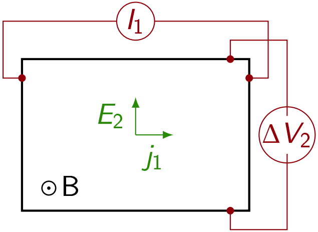

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Conductivity $\sigma_{12} := \frac{j_1}{E_2}$

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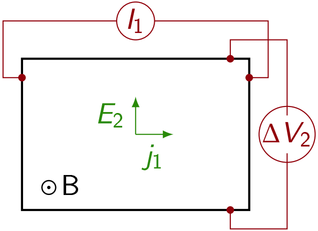

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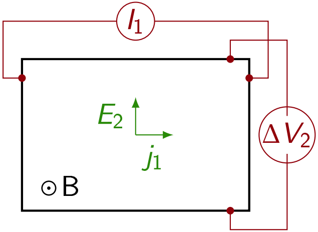

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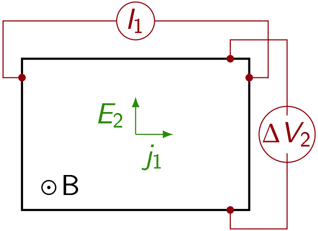

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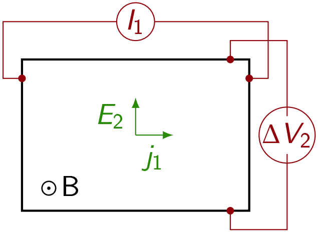

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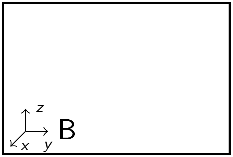

B: from spin-orbit coupling

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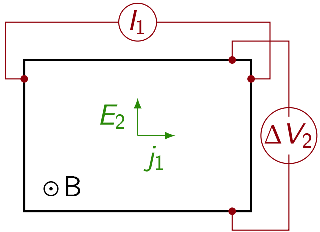

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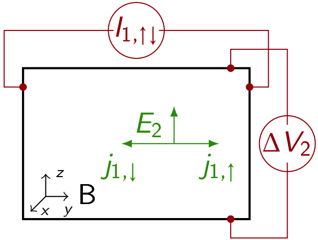

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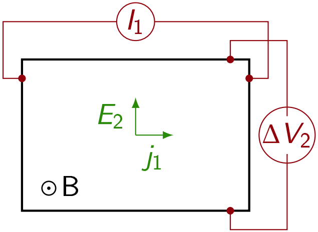

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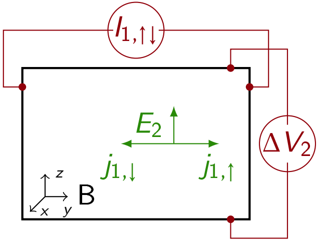

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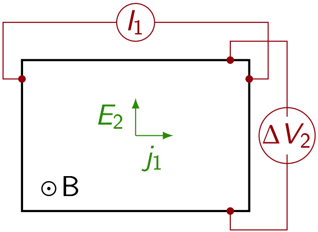

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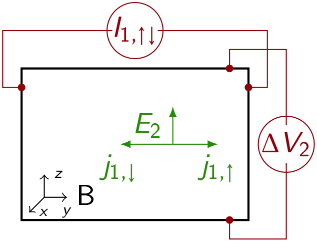

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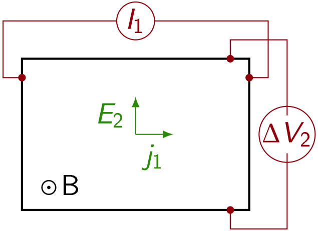

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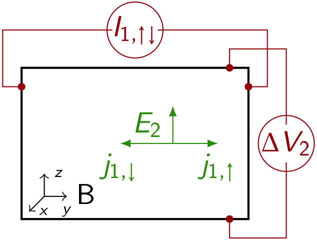

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Conductivity of an observable quantity

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Denoting by ρ_ε the state of the system after the perturbation has been turned on:

Q) *what is the change of the expectation value of an observable A caused by the perturbation εV at the leading order in its strength $\varepsilon \ll 1$?*

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Q) $$(H_0, \Pi_0, \varepsilon V) \quad \longrightarrow \quad \mathrm{Re}\,\tau(A\rho_\varepsilon) - \mathrm{Re}\,\tau(A\Pi_0) =: \varepsilon \cdot \sigma_A + o(\varepsilon)$$

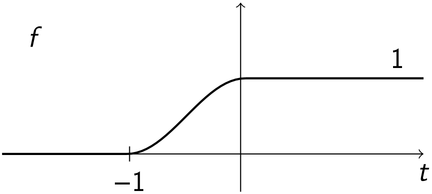
here A is an extensive observable, $\tau(\cdot)$ is the trace per unit volume and σ_A is called the conductivity of A.

A model for the switching process

Let

$$H^{\varepsilon}(t) := H_0 + \varepsilon f(t) V, \quad t \in I,$$

where $[-1,0] \subset I \subset \mathbb{R}$ is compact interval and $\varepsilon \ll 1$.



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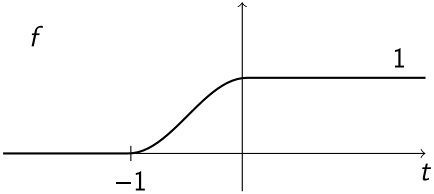

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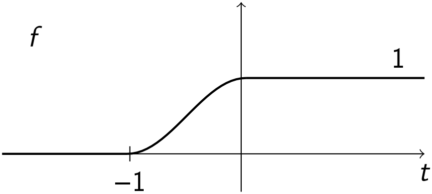

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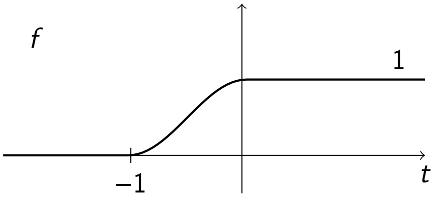

Let $\rho(t)$ the solution of the following Cauchy problem

$$\begin{cases} \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = [H^{\varepsilon}(\eta t), \rho(t)] \\ \rho(t_0) = \Pi_0 \ \forall\, t_0 \leq -1/\eta. \end{cases}$$

Then, $\rho(0)$ or $\rho(t)$ for any $t \geq 0$ is *"the natural candidate for the state* ρ_{ε} *of the system after the perturbation has been turned on".*

The usual paradigm for linear response

By the fundamental theorem of calculus, one obtains that $\rho_\varepsilon := \rho(0)$

$$\rho_\varepsilon = \Pi_0 + \mathrm{i}\varepsilon \int_{-\infty}^{0} \mathrm{d}t\, f(\eta t) \mathrm{e}^{\mathrm{i}tH_0} [X_j, \Pi_0] \mathrm{e}^{-\mathrm{i}tH_0} + \varepsilon^2 R^{\varepsilon,\eta,f},$$

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The existence and computation of the limit $\lim_{\eta\to 0^+} \widetilde{\sigma}^{\eta,\exp}$ for $A = J_i^{\mathrm{c}} := \mathrm{i}[H^\varepsilon(t), X_i]$ are proved *e. g.* for one-particle Hamiltonian in [Bellissard, van Elst, Schulz-Baldes JMP '98], [Aizenman, Graf JPA '98], [Bouclet, Germinet, Klein, Schenker JFA '05], [De Nittis, Lein Springer Briefs '17] $\cdots$

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Alternative approaches for transport properties of interacting many-body systems: [Fröhlich, Studer Rev. Mod. Phys. '93], [Jakšić, Ogata, Pillet CMP '06], [Giuliani, Mastropietro, Porta CMP '17] $\cdots$

A model for quantum transport

Assumption (H) on the unperturbed model

- $\mathscr{H} := L^2(\mathscr{X}) \otimes \mathbb{C}^N$,
  $\mathscr{X} = \mathbb{R}^d$ or $\mathscr{X} =$ discrete d-dimensional crystal $\subset \mathbb{R}^d$

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  - 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 $\mathscr{H}_{\mathrm{f}} := L^2(\mathscr{C}_1) \otimes \mathbb{C}^N$, $\mathscr{C}_1 := \mathscr{X}/\Gamma$

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  - Π_0 = Fermi projection on occupied bands below the spectral gap is in $\mathscr{B}_1^\tau$

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  -
    $$H_0 : \mathbb{R}^d \to \mathscr{L}(\mathscr{D}_{\mathrm{f}}, \mathscr{H}_{\mathrm{f}}), \quad k \mapsto H_0(k)$$

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

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Remark The above assumptions are satisfied

- in most tight-binding models having spectral gap (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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The S-current

Let $S = \mathrm{Id}_{L^2(\mathscr{X})} \otimes s$ be a selfadjoint operator

- The ***conventional*** S-current

$$J^S_{\mathrm{conv,i}} := \frac{1}{2}\left(\mathrm{i}S\,[H_0, X_i] + \mathrm{i}[H_0, X_i]\,S\right)$$

- The ***proper*** S-current

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- If $[H_0, S] = 0$ then $J^S_{\mathrm{conv,i}} \equiv J^S_{\mathrm{prop,i}}$
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$J^S_{\rm conv}$ versus $J^S_{\rm prop}$

Consider $s = s_z$

- $J^S_{\rm conv}$ adopted *e.g.* in [Schulz-Baldes CMP '13]:
  $J^S_{\rm conv}$ is periodic/covariant whenever H_0 is periodic/covariant but obviously it is not expressed as a full commutator with H_0

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First attempt: use Kubo's formula for spin transport

First one is tempted to use Kubo's formula

$$\sigma_A^{\mathrm{Kubo}} := \lim_{\eta \to 0^+} \widetilde{\sigma}^{\eta,\exp} = \lim_{\eta \to 0^+} \mathrm{i} \int_{-\infty}^{0} \mathrm{d}t\, \mathrm{e}^{\eta t} \tau(A \mathrm{e}^{\mathrm{i}tH_0} [X_j, \Pi_0] \mathrm{e}^{-\mathrm{i}tH_0}),$$

whose limit existence relies on two key properties of A: to be periodic ($\Rightarrow$ cyclicity of $\tau(\cdot)$) and to be a full commutator with H_0 ($\Rightarrow$ integration by parts).

But each of $J^S_{\mathrm{conv/prop}}$ has not both of these properties in the general case $[H_0, S] \neq 0 \Rightarrow$ Kubo's formula becomes cumbersome and intractable for the spin transport.

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A new paradigm for quantum transport theory: NEASS

We use a new paradigm for quantum transport theory, specially in linear response theory: construction of non-equilibrium almost-stationary state (NEASS) Π^{ε} such that for every $m \geq 1$

$$\sup_{\eta \in [\varepsilon^{m}, \varepsilon^{\frac{1}{m}}]} \left| \tau(A\rho(t)) - \tau(A\Pi^{\varepsilon}) \right| \leq C\varepsilon^{2}\left(1 + t^{d+1}\right), \quad \forall\, t \geq 0,$$

for "*suitable*" observable A.

This inequality is proved for interacting models on lattices [Henheik, Teufel arXiv '20, Teufel CMP '19, Monaco, Teufel RMP '19], while for one-body models in the continuum it is work in preparation with Teufel.

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Construction of the NEASS

Stationary perturbed model

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

Proposition

Under Assumption (H), there exists a unique NEASS such that

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where $\mathscr{L}_{H_0}^{-1}(\cdot)$ is the inverse Liouvillian, *i. e.* $[H_0, \mathscr{L}_{H_0}^{-1}(A)] = A$ for any $A = A^{\mathrm{OD}}$

Remark

Thanks to the gap condition, for any $A = A^{\mathrm{OD}}$

$$\mathscr{L}_{H_0}^{-1}(A) := \frac{\mathrm{i}}{2\pi}\oint_C \mathrm{d}z\,(H_0 - z\mathrm{Id})^{-1}\,[A, \Pi_0]\,(H_0 - z\mathrm{Id})^{-1}$$

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The conductivity of A by using the NEASS

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$\rightsquigarrow$

$$\sigma^S_{\mathrm{conv/prop,ij}} := \sigma_{J^S_{\mathrm{conv/prop,i}}} = \operatorname{Re}\tau(J^S_{\mathrm{conv/prop,i}}\Pi_1),$$

once it is proved that $\left|\tau(A\Pi_r^\varepsilon)\right| \leq C$, for $C > 0$ independent of ε

S-conductivity when $[H_0, S] \neq 0$

Theorem[G. M., G. Panati, S. Teufel]
Let $H^{\varepsilon} := H_0 - \varepsilon X_j$ with H_0 satisfying Assumption (H) and Π_1 given by the previous Proposition, then

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About the S-conductivity when $[H_0, S] \neq 0$

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For every $L \in 2\mathbb{N}+1$, we denote by

$$\mathscr{C}_L := \left\{ x \in \mathscr{X} : x = \sum_{j=1}^{d} \alpha_j a_j \text{ with } |\alpha_j| \leq L/2 \, \forall j \in \{1, \dots, d\} \right\}$$

where $\{a_1, \dots, a_d\}$ is a basis for the lattice Γ and $\chi_L := \chi_{\mathscr{C}_L}$.

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

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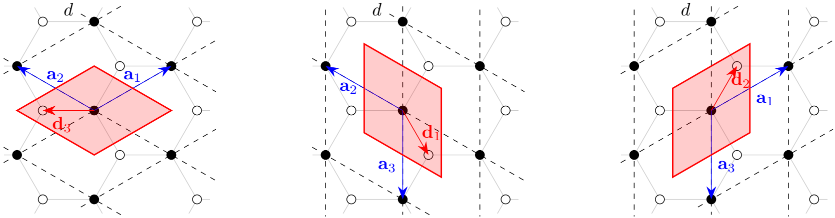
Unit fundamental cells

Examples for the honeycomb structure $\mathscr{X}$:



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Let $\mathscr{C}_1$ and $\widetilde{\mathscr{C}}_1$ be two unit cells. Then there exist a finite subset $I \subset \Gamma$ and a family of subsets $\{P_\gamma\}_{\gamma \in I} \subset \mathscr{X}$ such that

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Corollary

Let A be periodic and trace class on compact sets. Then

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About the S-conductivity when $[H_0, S] \neq 0$

Lemma

Let $\mathscr{C}_1$ and $\widetilde{\mathscr{C}}_1$ be two unit cells. Then there exist a finite subset $I \subset \Gamma$ and a family of subsets $\{P_\gamma\}_{\gamma \in I} \subset \mathscr{X}$ such that

$$\mathscr{C}_1 = \bigsqcup_{\gamma \in I} \mathrm{T}_\gamma P_\gamma \quad \text{and} \quad \widetilde{\mathscr{C}}_1 = \bigsqcup_{\gamma \in I} P_\gamma .$$

Corollary

Let A be periodic and trace class on compact sets. Then

- $\tau(A) = \widetilde{\tau}(A)$.
- In addition, if $\mathrm{Tr}(\chi_{P_\gamma} A \chi_{P_\gamma}) = 0$ for all $\gamma \in I$, then $\tau(X_i A) = \widetilde{\tau}(X_i A)$.

About the S-conductivity when $[H_0, S] \neq 0$

By virtue of the previous Corollary,

$$\text{if} \quad \mathrm{Tr}(\chi_{P_\gamma} \mathrm{i}[H_0, S]\Pi_1 \, \chi_{P_\gamma}) = 0 \quad \forall \gamma \in I$$

(*e. g.* if the model satisfies a *suitable* discrete rotational symmetry, as in the case of the Kane–Mele model),

then both $\sigma^S_{\mathrm{conv,ij}}$ and $\sigma^S_{\mathrm{prop,ij}}$ satisfy the *Unit Cell Consistency*

and, in particular in the discrete models

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

Main goal: Validity of the Kubo formula beyond linear response, *i. e.*

$$\tau(J\rho_\varepsilon) = \varepsilon\,\sigma_{\mathrm{Hall}} + \mathscr{O}(\varepsilon^\infty),$$

where $J := \mathrm{i}[H_0, X]$ is the charge current operator, ρ_ε denotes the state of the system after the perturbation has been turned on, and

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

Existing proofs of this statement, be it in the continuum [Klein, Seiler CMP '90] or discrete [Bachmann et al. AHP '21] setting for many-body electron gases, base on the physical *magnetic flux insertion argument* proposed by Laughlin [Laughlin PRB '81].

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A new paradigm for quantum transport theory: NEASS

We use a new paradigm for quantum transport theory, specially in linear response theory: construction of non-equilibrium almost-stationary state (NEASS) Π_n^ε such that for every $n, m \in \mathbb{N}$

$$\sup_{\eta \in [\varepsilon^m, \varepsilon^{\frac{1}{m}}]} \left| \tau(A\rho(t)) - \tau(A\Pi_n^\varepsilon) \right| \leq C\varepsilon^{n+1}\left(1 + t^{d+1}\right), \quad \forall\, t \geq 0 \qquad (\sharp)$$

for "*suitable*" observable A.

This inequality is proved for interacting models on lattices [Henheik, Teufel arXiv '20, Teufel CMP '19, Monaco, Teufel RMP '19], while for one-body models in the continuum it is work in preparation with Teufel.

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Construction of the NEASS at every order in ε

Stationary perturbed model

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

Theorem[G. M., D. Monaco]

Under Assumption (H), then for any $n \in \mathbb{N}$ there exists a unique NEASS such that

$$\Pi_n^{\varepsilon} := \mathrm{e}^{\mathrm{i}\varepsilon \mathscr{S}_n^{\varepsilon}} \Pi_0 \, \mathrm{e}^{-\mathrm{i}\varepsilon \mathscr{S}_n^{\varepsilon}} = \sum_{j=0}^{n} \varepsilon^j \Pi_j + \varepsilon^{n+1} \Pi_{\mathrm{reminder}}(\varepsilon)$$

where $\quad \mathscr{S}_n^{\varepsilon} := \sum_{j=1}^{n} \varepsilon^{j-1} A_j, \quad$ and $\quad [H^{\varepsilon}, \Pi_n^{\varepsilon}] = \varepsilon^{n+1} [R_n^{\varepsilon}, \Pi_n^{\varepsilon}].$

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

Theorem[G. M., D. Monaco]

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

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

where Π_n^{ε} is as in the statement of the previous Theorem and

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Remark

Thus, up to prove the validity of the NEASS approximation for the state of the system, after the perturbation has been switched on, in the sense of inequality ($\sharp$), the main goal is obtained.

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

Sketch of the proof

Let's recall $J\Pi_n^{\varepsilon} = \mathrm{i}[H_0, X]\Pi_n^{\varepsilon}$

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

Sketch of the proof

By using the cyclicity of $\tau(\cdot)$ and $(\Pi_n^\varepsilon)^2 = \Pi_n^\varepsilon$

$$\tau([H_0, X]\Pi_n^\varepsilon) = \tau(\Pi_n^\varepsilon[H^\varepsilon, X]\Pi_n^\varepsilon)$$

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

Sketch of the proof

In view of $[H^\varepsilon, \Pi_n^\varepsilon] = \varepsilon^{n+1}[R_n^\varepsilon, \Pi_n^\varepsilon]$

$$
\begin{aligned}
&\tau([H_0, X]\Pi_n^\varepsilon) = \tau(\Pi_n^\varepsilon[H^\varepsilon, X]\Pi_n^\varepsilon) \\
&= \tau([\Pi_n^\varepsilon H^\varepsilon \Pi_n^\varepsilon, \Pi_n^\varepsilon X \Pi_n^\varepsilon]) + \varepsilon^{n+1}\tau(\Pi_n^\varepsilon[[\Pi_n^\varepsilon, R_n^\varepsilon], [X, \Pi_n^\varepsilon]]\Pi_n^\varepsilon)
\end{aligned}
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Sketch of the proof

By using $H^\varepsilon := H_0 - \varepsilon Y$

$$
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&= \tau([\Pi_n^\varepsilon H_0 \Pi_n^\varepsilon, \Pi_n^\varepsilon X \Pi_n^\varepsilon]) - \varepsilon\,\tau([\Pi_n^\varepsilon Y \Pi_n^\varepsilon, \Pi_n^\varepsilon X \Pi_n^\varepsilon]) \\
&\quad + \varepsilon^{n+1}\,\tau(\Pi_n^\varepsilon[[\Pi_n^\varepsilon, R_n^\varepsilon], [X, \Pi_n^\varepsilon]]\Pi_n^\varepsilon)
\end{aligned}
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&\tau([H_0, X]\Pi_n^\varepsilon) = \tau(\Pi_n^\varepsilon[H^\varepsilon, X]\Pi_n^\varepsilon) \\
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&= \tau([\Pi_n^\varepsilon H_0 \Pi_n^\varepsilon, \Pi_n^\varepsilon X \Pi_n^\varepsilon]) - \varepsilon\,\tau([\Pi_n^\varepsilon Y \Pi_n^\varepsilon, \Pi_n^\varepsilon X \Pi_n^\varepsilon]) \\
&\quad + \varepsilon^{n+1}\tau(\Pi_n^\varepsilon[[\Pi_n^\varepsilon, R_n^\varepsilon], [X, \Pi_n^\varepsilon]]\Pi_n^\varepsilon)
\end{aligned}
$$

We conclude noticing that $\tau([\Pi_n^\varepsilon H_0 \Pi_n^\varepsilon, \Pi_n^\varepsilon X \Pi_n^\varepsilon]) = 0$ by cyclicity of the trace, and the *Chern–Simons-like formula* defining $P_U := UPU^{-1}$ $\tau([P_U X P_U, P_U Y P_U]) = \tau([PXP, PYP])$ for U, P periodic and *regular enough*.

Thank you for your attention!