Non-equilibrium almost-stationary states and linear response for gapped non-interacting quantum systems

Giovanna Marcelli
joint works with D. Monaco (*Roma Tre*, Roma), G. Panati (*La Sapienza*, Roma), and S. Teufel (*Eberhard-Karls*, Tübingen)

[MaMoPT]: soon on arXiv and [MaT]: in progress

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Introduction

Barry Simon: *Fifteen problems in mathematical physics* (1984)

4. Transport Theory: At some level, the fundamental difficulty of transport theory is that it is a steady state rather than equilibrium problem, so that the powerful formalism of equilibrium statistical mechanics is unavailable, and one does not have any way of precisely identifying the steady state and thereby computing things in it.

$$\vdots$$

Problem 4 B (Kubo Formula): Either justify Kubo's formula in a quantum model, or else find an alternate theory of conductivity.

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Q1) *How does a system described by a Hamiltonian H_0 that is initially in an equilibrium state Π_0 respond to a small static perturbation εV?*

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here ρ_ε denotes the state of the system after the perturbation has been turned on

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Q2) *What is the change of the expectation value of an observable A caused by the perturbation εV at the leading order in its strength $\varepsilon \ll 1$?*

$$(H_0, \Pi_0, \varepsilon V) \quad \longrightarrow \quad \mathrm{Re}\,\mathscr{T}(A\rho_\varepsilon) - \mathrm{Re}\,\mathscr{T}(A\Pi_0) =: \varepsilon \cdot LR_A + o(\varepsilon)$$

here $\mathscr{T}(\cdot)$ denotes a trace-like functional and LR_A is called the linear response coefficient for A

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Q2) $$(H_0, \Pi_0, \varepsilon V) \longrightarrow \mathrm{Re}\,\mathrm{Tr}(A\rho_\varepsilon) - \mathrm{Re}\,\mathrm{Tr}(A\Pi_0) =: \varepsilon \cdot G_A + o(\varepsilon)$$

here A is an intensive observable, $\mathrm{Tr}(\cdot)$ is the standard trace and G_A is called the conductance for A

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

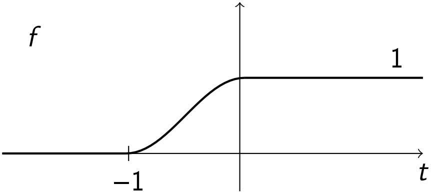
here A is an extensive observable, $\tau(\cdot)$ is the trace per unit volume and σ_A is called the conductivity for A

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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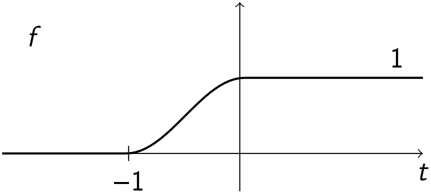

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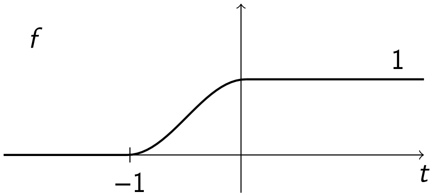

Let $\rho(t)$ the solution of the following Cauchy problem

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

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"*.

Kubo's formula

By the Fundamental Theorem of Calculus, one obtains that $\rho_\varepsilon := \rho(0)$

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

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and thus

$$\tau(A\rho_\varepsilon) = \tau(A\Pi_0) + \varepsilon \cdot \widetilde{\sigma}^{\eta,f} + \tau(AR^{\varepsilon,\eta,f})$$

with

$$\widetilde{\sigma}^{\eta,f} := -\mathrm{i} \int_{-\infty}^{0} \mathrm{d}t\, f(\eta t) \tau(A \mathrm{e}^{\mathrm{i}tH_0} [V, \Pi_0] \mathrm{e}^{-\mathrm{i}tH_0}).$$

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Now, choosing $f = \exp$ and taking the adiabatic limit $\eta \to 0^+$, one gets Kubo's formula for the linear response coefficient

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

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"Justifying Kubo's formula" has two different meanings:

M1) Show existence of the limit and compute $\lim_{\eta \to 0^+} \widetilde{\sigma}^{\eta,\exp}$

M2) Show that $\tau(AR^{\varepsilon,\eta,f}) = o(\varepsilon)$ uniformly in η and compute $\lim_{\eta \to 0^+} \widetilde{\sigma}^{\eta,f} = \sigma_A^{\mathrm{Kubo}}$ for any switching function f

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NEASS method

Circumnavigating the time-adiabatic perturbation method, our main goal is

$\widetilde{\mathbf{M2}}$) Construct the non-equilibrium almost-stationary state (NEASS) Π_n^ε such that

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

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$\rightsquigarrow$ A is the current operator (for *local* observables, it is proved in the setting of interacting models on lattices [Teufel CMP '19]. A *similar* statement is shown for quantum spin systems in [Bachmann, De Roeck, Fraas CMP'18] for $f = \exp$, and for the conductance and $\varepsilon = \eta$ in [Elgart, Schlein CPAM '04]).

A model for quantum transport

Continuous model: $\mathscr{H} := L^2(\mathbb{R}^d)$

Assumption (**H**) on the unperturbed model

(**H1**) $H_0 := \frac{1}{2}(-\mathrm{i}\nabla - \mathbf{A}(x))^2 + V(x)$ on $C_c^\infty(\mathbb{R}^d)$,
where $\mathbf{A}$ and V satisfy the Leinfelder–Simader conditions

(**H2**) H_0 admits a spectral gap $\mathscr{G}$

Remark

- (**H1**) $\Longrightarrow$ H_0 is essentially self-adjoint on $C_c^\infty(\mathbb{R}^d)$ and bounded from below
- (**H2**) $\Longrightarrow$ The Fermi projection $\Pi_0 = \frac{\mathrm{i}}{2\pi}\oint_{C_\mu} \mathrm{d}\lambda\,(H_0 - \lambda \mathrm{Id})^{-1}$, $\mu \in \mathscr{G}$
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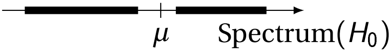

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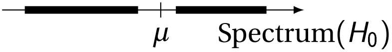

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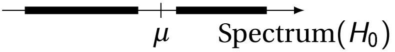

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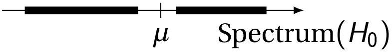

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A model for quantum transport

Perturbed model

We want to model a time-dependent spatially uniform electric field $\mathbf{E}(t)$ of small intensity, induced in the j-th direction and switched on slowly in time $\rightsquigarrow$ $\varepsilon, \eta \in (0,1]$

$$H^{\varepsilon}(\eta t) := H_0 - \varepsilon f(\eta t) X_j, \quad \eta t \in I,$$

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⚠ $H^{\varepsilon}(\eta t)$ is *not* gapped for $\eta t \geq 0$.

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- Π_n^ε almost-commutes with the stationary perturbed Hamiltonian $H^\varepsilon := H_0 - \varepsilon X_j$, namely $[H^\varepsilon, \Pi_n^\varepsilon] = \mathscr{O}(\varepsilon^{n+1})$

Mathematical framework

For $\alpha > 0$,

$$F_\alpha(x) := \frac{\mathrm{e}^{-\alpha|x|}}{(1+|x|)^{d+1}} \text{ for every } x \in \mathbb{R}^d$$

$$\mathscr{B}_\alpha := \left\{ A \in \mathscr{L}(\mathscr{H}_c, \mathscr{H}) : \exists\ C_A > 0 \mid \left\| \chi_x A \chi_y \right\| \le C_A F_\alpha(x-y) \quad \forall x, y \in \mathbb{Z}^d \right\}$$

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Construction of the NEASS

Theorem[M., Teufel]

Let $H^\varepsilon := H_0 - \varepsilon X_j$, where H_0 enjoys Assumption (H). Then $\exists$ a sequence $\{A_j\}_{j\in\mathbb{N}} \in \widetilde{\mathscr{B}}_{\alpha_1}$, $\alpha_1 > 0$ such that $\forall n \in \mathbb{N}$ the NEASS is uniquely defined as

$$\Pi_n^\varepsilon = \mathrm{e}^{\mathrm{i}\varepsilon S_n^\varepsilon}\Pi_0\mathrm{e}^{-\mathrm{i}\varepsilon S_n^\varepsilon} = \sum_{j=0}^{n} \varepsilon^j \Pi_j + \varepsilon^{n+1}\Pi_r^\varepsilon \in \widetilde{\mathscr{B}}_{\alpha_2},$$

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S-conductivity

Theorem[M., Monaco, Panati, Teufel]

Let $\mathscr{H} := L^2(\mathbb{R}^d) \otimes \mathbb{C}^N$. Let H_0 satisfy Assumption $\widetilde{(\mathbf{H1})}$ (*i. e.* periodicity + *mild technical hypotheses*) and $(\mathbf{H2})$.

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Let $\mathscr{H} := L^2(\mathbb{R}^d) \otimes \mathbb{C}^N$. Let H_0 satisfy Assumption $\widetilde{(\mathbf{H1})}$ (*i. e.* periodicity + *mild technical hypotheses*) and $(\mathbf{H2})$.
Let $J_i := \mathrm{i}\,[H_0, S\,X_i]$, where $S = \mathrm{Id}_{L^2(\mathbb{R}^d)} \otimes s$ is a self-adjoint operator.

- $s = \mathrm{Id} \longrightarrow$ charge current (QHE);
- $s = s_z = \sigma_z/2 \longrightarrow$ spin current (QSHE) proposed by [Shi, Zhang, Xiao, Niu PRL '06] and adopted in [M., Panati, Tauber AHP '19].

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Then

$$\sigma^{\varepsilon}_{ij} = \underbrace{\mathrm{i}\tau\Big([[SX_i,\Pi_0],[X_j,\Pi_0]]\Pi_0\Big)}_{=:\text{Chern-like term}} +$$

$$\underbrace{\mathrm{Re}\,\tau\Big(\mathrm{i}[H_0,(SX_i)^{\mathrm{D}}]\Pi_1 + \mathrm{i}[H_0,(SX_i)^{\mathrm{OD}}\Pi_1] + \mathrm{i}[[SX_i,\Pi_0],\Pi_0[\Pi_0,X_j]]\Big)}_{=:\text{beyond-Chern-like terms}}$$

$$+\,O(\varepsilon).$$

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Let $J_i := \mathrm{i}\,[H_0, S\,X_i]$.
In addition, if $[H_0, S] = 0$ then

$$\begin{aligned} \sigma_{ij}^{\varepsilon} &= \mathrm{i}\tau\Big(S\Pi_0\big[\,[X_i,\Pi_0],[X_j,\Pi_0]\,\big]\Big) + O(\varepsilon) \\ &= \frac{\mathrm{i}}{(2\pi)^d}\int_{\mathbb{B}^d} \mathrm{d}k\ \mathrm{Tr}_{\mathscr{H}_{\mathrm{f}}}\Big(S\,\Pi_0(k)\,\big[\partial_{k_j}\Pi_0(k), \partial_{k_i}\Pi_0(k)\big]\Big) + O(\varepsilon). \end{aligned}$$

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Remark *conditional* cyclicity of $\tau(\cdot)$ $\Longrightarrow$ the beyond-Chern-like terms vanish. In $d = 2$ the Chern-like 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).

S-conductivity

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$$= \frac{\mathrm{i}}{(2\pi)^d} \int_{\mathbb{B}^d} \mathrm{d}k \, \mathrm{Tr}_{\mathscr{H}_{\mathrm{f}}}\Big(S\,\Pi_0(k)\left[\partial_{k_j}\Pi_0(k), \partial_{k_i}\Pi_0(k)\right]\Big) + O(\varepsilon).$$

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

Ongoing part

- Justification of the validity of the linear response using NEASS method (*finite speed of propagation estimates* / *Lieb–Robinson bound type estimates* are needed).
- Study higher-order corrections in ε to the formula for the S-conductivity $\sigma_{ij}^{\varepsilon}$.