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

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1. Interacting fermions on the lattice

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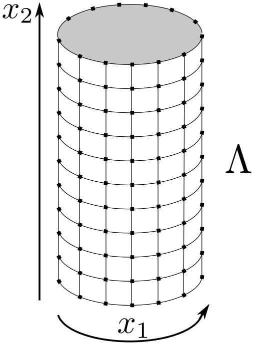

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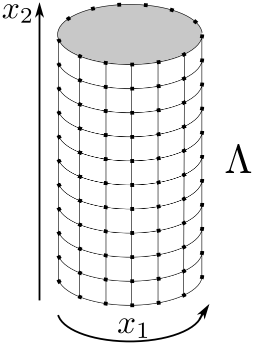

The N-particle Hilbert space for such a system is $\mathfrak{h}_{\Lambda,N} := \ell^2(\Lambda, \mathbb{C}^s)^{\wedge N}$ and it will be convenient to work on Fock space $\mathfrak{F}_\Lambda := \bigoplus_{N=0}^{s|\Lambda|} \mathfrak{h}_{\Lambda,N}$.

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A typical Hamiltonian could be of the form

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\begin{aligned}
H_0^\Lambda &= \sum_{(x,y)\in\Lambda^2} a_x^* \, T(x \overset{\Lambda}{-} y) \, a_y + \sum_{x\in\Lambda} a_x^* \phi(x) a_x \\
&+ \sum_{(x,y)\in\Lambda^2} a_x^* a_x \, W(x \overset{\Lambda}{-} y) \, a_y^* a_y - \mu \, \mathfrak{N}_\Lambda \,,
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where a_x^* and a_x are standard fermionic creation and annihilation operators of fermions at the sites $x \in \Lambda$.

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In the following by a "quasi-local operator family" we mean a family $A = \{A^\Lambda\}$ of self-adjoint operators A^Λ indexed by the domain Λ and possibly other parameters that is a "sum of local terms". Typically

$$\|A^\Lambda\| \sim |\Lambda| = L^d\,.$$

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Gap assumption

We assume that smallest eigenvalue E_0^Λ (ground state) of $H_0 = \{H_0^\Lambda\}$ is separated from the rest of the spectrum uniformly in the volume $|\Lambda|$,

$$\inf_\Lambda \operatorname{dist}\left(E_0^\Lambda, \sigma(H_0^\Lambda) \setminus \{E_0^\Lambda\}\right) =: g > 0\,.$$

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Examples

- Electrons of an insulating material, i.e. with the chemical potential μ in a “band gap”.
- The filled Dirac sea.

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One is interested in the response of the system to a "small" ($\varepsilon \ll 1$) perturbation $V^{\varepsilon,\Lambda}$, when initially the system starts in its ground state ρ_0^Λ.

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Then, in general,

$$H^{\varepsilon,\Lambda} := H^\Lambda + V^{\varepsilon,\Lambda}$$

no longer has a gapped ground state and the question arises:

What is the state of the system after we turned on the perturbation?

2. Linear response

Adiabatic switching: Let

$$H^{\varepsilon,\Lambda}(t) := H^\Lambda + f(t)\, V^{\varepsilon,\Lambda}$$

with a switch function $f : \mathbb{R} \to \mathbb{R}$ such that $f(t) = 0$ for $t \leq -1$ and $f(t) = 1$ for $t \geq 0$.

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Let $\rho^{\varepsilon,\Lambda,\eta}(t)$ be the solution of the time-dependent Schrödinger equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\rho^{\varepsilon,\Lambda,\eta,f}(t) = [H^{\varepsilon,\Lambda}(\eta t), \rho^{\varepsilon,\Lambda,\eta,f}(t)]$$

with $\rho^{\varepsilon,\Lambda,\eta,f}(t) = \rho_0^{\Lambda}$ for $t \leq -1/\eta$ and adiabatic parameter $\eta \ll 1$.

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with $\rho^{\varepsilon,\Lambda,\eta,f}(t) = \rho_0^\Lambda$ for $t \leq -1/\eta$ and adiabatic parameter $\eta \ll 1$.

Let O be a local observable or B^Λ an extensive observable, then one is interested in the expectations at time $t = 0$ when the perturbation is fully switched on,

$$\langle O \rangle_{\rho^{\varepsilon,\Lambda,\eta,f}(0)} := \mathrm{tr}(\rho^{\varepsilon,\Lambda,\eta,f}(0)\, O)$$

resp.

$$\langle B \rangle_{\rho^{\varepsilon,\Lambda,\eta,f}(0)} := \tfrac{1}{|\Lambda|}\, \mathrm{tr}(\rho^{\varepsilon,\Lambda,\eta,f}(0)\, B^\Lambda)\,.$$

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- To avoid finite size effects, one would like to take the thermodynamic limit $\Lambda \to \mathbb{Z}^d$.
- One expects that in the adiabatic limit $\eta \to 0$ the expressions become independent of the form f of the switching process.
- One expects simple managable expressions for the first order Taylor coefficient of the response in an expansion in powers of the strength $\varepsilon \ll 1$ of the perturbation $V^{\varepsilon,\Lambda}$.

2. Linear response

I.e. one is interested in the asymptotic expansion of

$$\lim_{\eta \to 0} \lim_{\Lambda \to \mathbb{Z}^d} \langle O \rangle_{\rho^{\varepsilon,\Lambda,\eta,f}(0)} = O_0 + \varepsilon O_1 + o(\varepsilon)\,.$$

The coefficient O_1 is called the linear response coefficient.

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In the standard derivation of Kubo's formula for O_1 one approximates $\rho^{\varepsilon,\Lambda,\eta,f}(0)$ by first order time-dependent perturbation theory

$$\rho^{\varepsilon,\Lambda,\eta,f}(0) = \rho_0^\Lambda + \mathrm{i}\int_{-\infty}^{0} f(\eta t)\,\mathrm{e}^{\mathrm{i}H_0^\Lambda t}\,[V^{\varepsilon,\Lambda},\rho_0^\Lambda]\,\mathrm{e}^{-\mathrm{i}H_0^\Lambda t}\,\mathrm{d}t + R^{\varepsilon,\Lambda,\eta,f}\,.$$

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Kubo's formula for the linear response coefficient is then

$$\widetilde{O}_1 := \lim_{\varepsilon\to 0}\lim_{\eta\to 0}\lim_{\Lambda\to\mathbb{Z}^d}\frac{\mathrm{i}}{\varepsilon}\int_{-\infty}^{0} f(\eta t)\,\left\langle\left[V^{\varepsilon,\Lambda},\mathrm{e}^{-\mathrm{i}H_0^\Lambda t}\,O\mathrm{e}^{\mathrm{i}H_0^\Lambda t}\right]\right\rangle_{\rho_0^\Lambda}\mathrm{d}t\,.$$

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Justifying Kubo's formula means to show that O_1 is well defined and that it agrees with $\widetilde{O}_1$, i.e. that

$$\sup_\eta\sup_\Lambda\mathrm{tr}(R^{\varepsilon,\Lambda,\eta,f}\,O) = o(\varepsilon).$$

3. Rigorous result for interacting systems with open gap

If $H^{\varepsilon,\Lambda}(t)$ remains gapped for all $t \in (-\infty, 0]$ then, according to the adiabatic theorem,

$$\lim_{\eta \to 0} \rho^{\varepsilon,\Lambda,\eta,f}(0) = \rho_0^{\varepsilon,\Lambda}$$

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Recently **Bachmann, De Roeck, and Fraas** proved an adiabatic theorem for interacting spin systems with error bounds that are uniform in the system size Λ,

$$\mathrm{tr}\left(\left(\rho^{\varepsilon,\Lambda,\eta,f}(0) - \rho_0^{\varepsilon,\Lambda}\right) O\right) \lesssim \eta \, .$$

4. Non-equilibrium almost-stationary states

How does the solution $\rho^{\varepsilon,\Lambda,\eta}(t)$ of the time-dependent Schrödinger equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\rho^{\varepsilon,\Lambda,\eta,f}(t) = [H^{\varepsilon,\Lambda}(\eta t), \rho^{\varepsilon,\Lambda,\eta,f}(t)]$$

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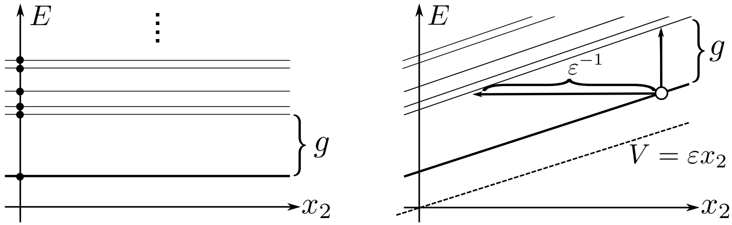

4. Non-equilibrium almost-stationary states

Theorem 1: Construction of the NEASS

Let

$$H^\varepsilon = H_0 + V^\varepsilon + \varepsilon H_1\,,$$

where H_0, H_1 are quasi-local operator families, V^ε is a slowly varying potential, and H_0 satisfies the gap assumption.

Then there is a sequence of self-adjoint quasi-local operator-families $(A_\mu)_{\mu\in\mathbb{N}}$, such that for any $n \in \mathbb{N}$ it holds that the projector

$$\Pi_n^{\varepsilon,\Lambda} := \mathrm{e}^{\mathrm{i}\varepsilon S_n^{\varepsilon,\Lambda}}\, P_0^\Lambda \mathrm{e}^{-\mathrm{i}\varepsilon S_n^{\varepsilon,\Lambda}} \quad \text{with} \quad S_n^{\varepsilon,\Lambda} := \sum_{\mu=1}^{n} \varepsilon^{\mu-1} A_\mu^{\varepsilon,\Lambda}$$

satisfies

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

for some quasi-local operator-family R_n^ε.

4. Non-equilibrium almost-stationary states

Quasi-locality of the generator $S^{\varepsilon,\Lambda}$ is important, because for local observables O we then have

$$\mathrm{tr}\left(\Pi_n^{\varepsilon,\Lambda}\, O\right) = \mathrm{tr}\left(\mathrm{e}^{\mathrm{i}\varepsilon S_n^{\varepsilon,\Lambda}}\, P_0^\Lambda \mathrm{e}^{-\mathrm{i}\varepsilon S_n^{\varepsilon,\Lambda}}\, O\right) = \mathrm{tr}\Big(P_0^\Lambda\, \underbrace{\mathrm{e}^{-\mathrm{i}\varepsilon S_n^{\varepsilon,\Lambda}}\, O\, \mathrm{e}^{\mathrm{i}\varepsilon S_n^{\varepsilon,\Lambda}}}_{\text{almost local}}\Big)\,,$$

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Quasi-locality of the remainder term $R_n^{\varepsilon,\Lambda}$ is important, because this allows to prove "almost invariance" of the state $\Pi_n^{\varepsilon,\Lambda}$ in the following sense:

Let $\rho^{\varepsilon,\Lambda}(t)$ be the solution of the Schrödinger equation

$$\mathrm{i}\tfrac{\mathrm{d}}{\mathrm{d}t}\, \rho^{\varepsilon,\Lambda}(t) = [H^{\varepsilon,\Lambda}, \rho^{\varepsilon,\Lambda}(t)] \qquad \text{with} \qquad \rho^{\varepsilon,\Lambda}(0) = \Pi_n^{\varepsilon,\Lambda}\,.$$

Then there exists a constant C such that for any local observable O

$$\sup_\Lambda \left| \langle O \rangle_{\rho^{\varepsilon,\Lambda}(t)} - \langle O \rangle_{\Pi_n^{\varepsilon,\Lambda}} \right| \leq C\, \varepsilon^{n-d+1}\, |t|(1+|t|^d)\, \|O\|\,.$$

5. Adiabatic switching

Theorem 2: Adiabatic Switching and the NEASS

Let $H = H_0 + V_v + \varepsilon H_1$ as in the previous theorem. Let $f : \mathbb{R} \to \mathbb{R}$ be a smooth "switching" function with $f(t) = 0$ for $t \leq -1$ and $f(t) = 1$ for $t \geq 0$, and define $H(t) := H_0 + f(t)(V_v + \varepsilon H_1)$. Let $\rho^{\varepsilon,\Lambda,\eta,f}(t)$ be the solution of the adiabatic time-dependent Schrödinger equation

$$\mathrm{i}\,\eta \tfrac{\mathrm{d}}{\mathrm{d}t}\, \rho^{\varepsilon,\Lambda,\eta,f}(t) = [H^{\varepsilon,\Lambda}(t), \rho^{\varepsilon,\Lambda,\eta,f}(t)]$$

with adiabatic parameter $\eta \leq \varepsilon$ and initial datum $\rho^{\varepsilon,\Lambda,\eta,f}(t) = P_*^\Lambda$ for all $t \leq -1$.

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Then for any $n \in \mathbb{N}$ there exists a constant C such that for any local observable O and for all $t \geq 0$

$$\sup_\Lambda \left| \langle O \rangle_{\rho^{\varepsilon,\Lambda,\eta,f}(t)} - \langle O \rangle_{\Pi_n^{\varepsilon,\Lambda}} \right| \leq C\, \frac{\varepsilon^{n-d+1}}{\eta}\, t(1 + t^d)\, \|O\| \,,$$

where $\Pi_n^{\varepsilon,\Lambda}$ is the NEASS of $H^{\varepsilon,\Lambda}$ constructed in Theorem 1.

Theorem 3: (Linear) Response

For a local observable O define the response as

$$\sigma^{\varepsilon,\Lambda,\eta,f}(t) := \left(\langle O \rangle_{\rho^{\varepsilon,\Lambda,\eta,f}(t)} - \langle O \rangle_{P_0^\Lambda} \right) ,$$

and for $j \in \mathbb{N}$ the jth order response coefficient as $\sigma_j^\Lambda := \langle \mathcal{K}_j^\varepsilon[O] \rangle_{P_0^\Lambda}$, where the $\mathcal{K}_j^{\varepsilon,\Lambda}$'s are explicit maps given by iterated commutators with quasi-local operators, in particular,

$$\langle \mathcal{K}_1^\varepsilon[O] \rangle_{P_0^\Lambda} = \langle [[R_0, V^\varepsilon], O] \rangle_{P_0^\Lambda} .$$

6. Linear and higher order response

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$$\sigma^{\varepsilon,\Lambda,\eta,f}(t) := \left(\langle O \rangle_{\rho^{\varepsilon,\Lambda,\eta,f}(t)} - \langle O \rangle_{P_0^\Lambda} \right) ,$$

and for $j \in \mathbb{N}$ the jth order response coefficient as $\sigma_j^\Lambda := \langle \mathcal{K}_j^\varepsilon [O] \rangle_{P_0^\Lambda}$, where the $\mathcal{K}_j^{\varepsilon,\Lambda}$'s are explicit maps given by iterated commutators with quasi-local operators, in particular,

$$\langle \mathcal{K}_1^\varepsilon [O] \rangle_{P_0^\Lambda} = \langle [[R_0, V^\varepsilon] , O] \rangle_{P_0^\Lambda} .$$

Then for any $n, m \in \mathbb{N}$ there exists a constant $C \in \mathbb{R}$ independent of ε, such that for $t \geq 0$ and $r = \max\{2d, n+1\}$

$$\sup_\Lambda \sup_{\eta \in [\varepsilon^m, \varepsilon]} \left| \sigma^{\varepsilon,\Lambda,\eta,f}(t) - \sum_{j=1}^{n} \varepsilon^j \sigma_j^\Lambda \right| \leq \varepsilon^{n+1} \, C \, (1 + t^{d+1}) \, \|O\| \, .$$

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- The admissible time scales η of the adiabatic switching are coupled to the strength of the perturbation: the switching must be slow relative to the strength of the perturbation, i.e. $\eta \lesssim \varepsilon$, but sufficiently fast relative to the life-time of the NEASS, i.e. $\varepsilon^m \lesssim \eta$ for some $m \in \mathbb{N}$.

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Thanks for your attention!

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