Adiabatic theorems and linear response in the thermodynamic limit

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Linear response and Kubo's formula

In the context of Hamiltonian quantum systems, the linear response formalism answers the following question:

How does a system described by a Hamiltonian H_0 that is initially in an equilibrium state ρ_0 respond to a small static perturbation εV?

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Or somewhat more precisely:

What is the change

$$\mathrm{tr}(\rho_\varepsilon A) - \mathrm{tr}(\rho_0 A) = \varepsilon \cdot \sigma_A + o(\varepsilon)$$

of the expectation value of an observable A caused by the perturbation εV at leading order in its strength ε ?

Here ρ_ε denotes the state of the system after the perturbation has been turned on and σ_A is called the linear response coefficient for A.

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The answer clearly hinges on the problem of determining ρ_ε.

Motivation and plan of the talk

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.*

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Plan of the talk:

1. Linear response at zero temperature: setup and ideas
2. Adiabatic theorem for fermions in the thermodynamic limit with a gap in the bulk

Linear response and Kubo's formula

Modelling the switching process: Let

$$H_\varepsilon(t) := H_0 + f(t)\,\varepsilon V$$

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 $\rho(t)$ be the solution of the time-dependent Schrödinger equation

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

with $\rho(t) = \rho_0$ for $t \leq -1/\eta$ and adiabatic parameter $\eta \ll 1$.

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with $\rho(t) = \rho_0$ for $t \leq -1/\eta$ and adiabatic parameter $\eta \ll 1$.

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

Linear response and Kubo's formula

Approximating $\rho_\varepsilon := \rho(0)$ by first order time-dependent perturbation theory

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

one obtains

$$\mathrm{tr}(\rho_\varepsilon A) - \mathrm{tr}(\rho_0 A) = \varepsilon\,\tilde{\sigma}_A^{\eta,f} + \mathrm{tr}(R^{\varepsilon,\eta,f} A)$$

with

$$\tilde{\sigma}_A^{\eta,f} = \mathrm{i}\int_{-\infty}^{0} f(\eta t)\,\left\langle \left[V, \mathrm{e}^{-\mathrm{i}H_0 t}\,A\,\mathrm{e}^{\mathrm{i}H_0 t}\right]\right\rangle_{\rho_0}\mathrm{d}t\,.$$

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$$\sigma_A^{\mathrm{Kubo}} := \lim_{\eta\to 0}\tilde{\sigma}_A^{\eta,\exp} = \lim_{\eta\to 0}\mathrm{i}\int_{-\infty}^{0}\mathrm{e}^{\eta t}\,\left\langle\left[V,\mathrm{e}^{-\mathrm{i}H_0 t}\,A\,\mathrm{e}^{\mathrm{i}H_0 t}\right]\right\rangle_{\rho_0}\mathrm{d}t\,.$$

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- Show existence of the limit and compute $\sigma_A^{\mathrm{Kubo}} = \lim_{\eta \to 0} \tilde{\sigma}_A^{\eta,\exp}$.

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  (e.g. **Bouclet, Germinet, Klein, Schenker** *JFA* '05)

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"Justifying Kubo's formula" can mean two different things now:

- Show existence of the limit and compute $\sigma_A^{\mathrm{Kubo}} = \lim_{\eta\to 0} \tilde{\sigma}_A^{\eta,\exp}$.
- Show that $\mathrm{tr}(R^{\varepsilon,\eta,f} A) = o(\varepsilon)$ uniformly in η and that $\sigma_A^{\mathrm{Kubo}} = \lim_{\eta\to 0} \tilde{\sigma}_A^{\eta,f}$ for any switching function f.

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For a quantum system with Hamiltonian H_0 starting in the gapped ground state ρ_0 scenario (a) occurs, whenever the perturbation does not close the spectral gap.

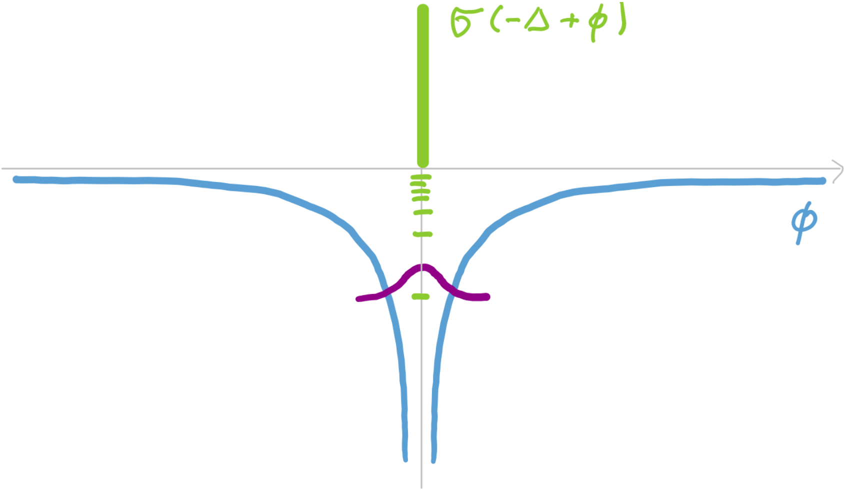
Then, according to the adiabatic theorem, the state $\rho(t)$ for times $t \geq 0$, i.e. when the perturbation is fully switched on, is

$$\rho_\varepsilon = \rho_0^\varepsilon + \mathcal{O}(\varepsilon)\,,$$

where ρ_0^ε denotes the ground state of the perturbed Hamiltonian H_ε.

(e.g. **Elgart, Schlein** *CPAM* '04; **Bachmann et al.** *CMP* '18)

Example for (b): The Stark Hamiltonian



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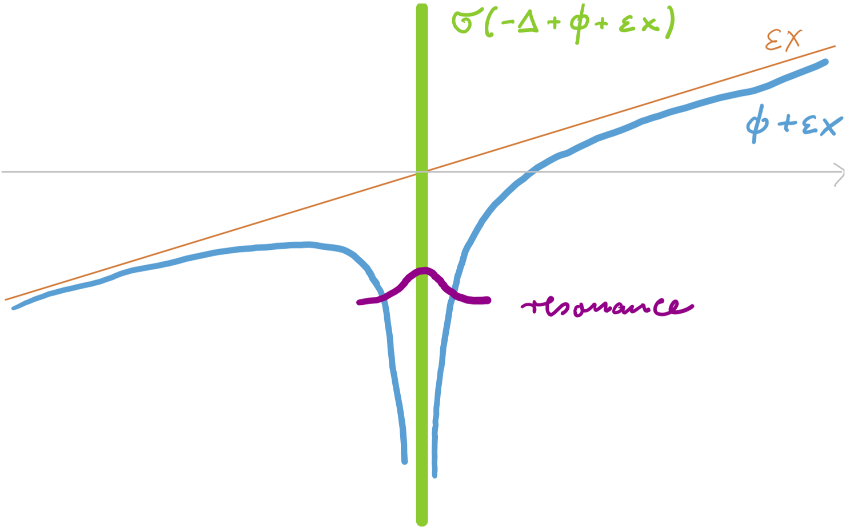

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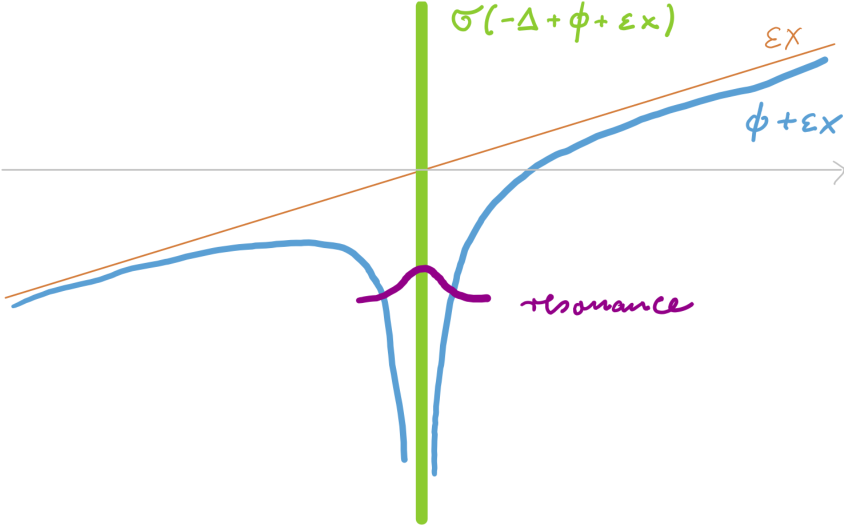

e.g. **Abou Salem, Fröhlich** *CMP* '07, **Elgart, Hagedorn** *CPAM* '11.

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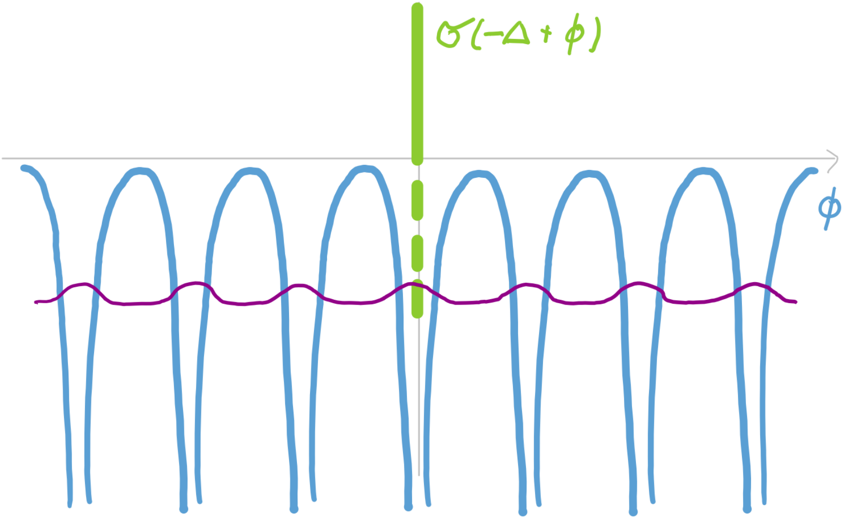

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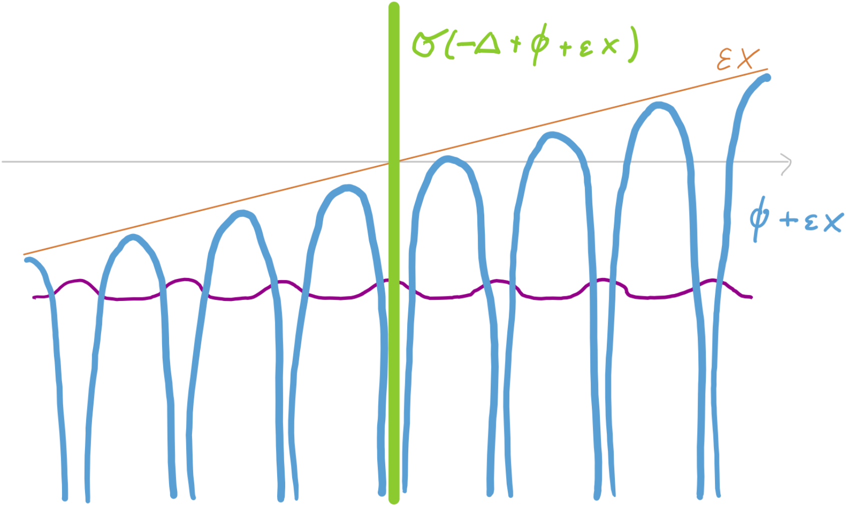

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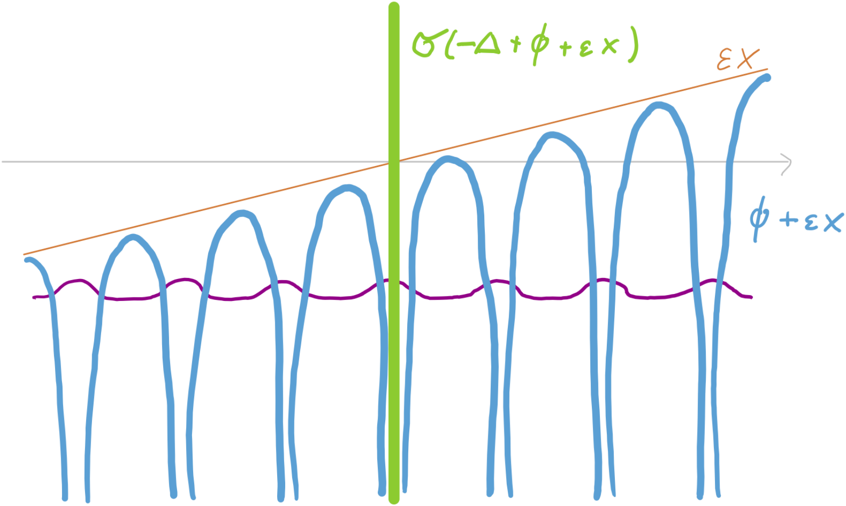

Nenciu *JMP* '02; **Panati, Spohn, T.** *CMP* '03.

Interacting fermions on the lattice

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The algebra $\mathcal{L}(\mathfrak{F}_X)$ of bounded operators on $\mathfrak{F}_X$ is generated by the fermionic creation and annihilation operators $a^*_{x,i}$ and $a_{x,i}$.
By $\mathcal{A}_X \subset \mathcal{L}(\mathfrak{F}_X)$ we denote the sub-algebra of operators that commute with the number operator $\mathfrak{N}^X := \sum_{x \in X} a^*_{x,i} a_{x,i}$.

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A typical physical Hamiltonian is of the form

$$\begin{aligned} H_0^X \;&=\; \sum_{(x,y)\in X^2} a^*_{x,i}\, T^X_{ij}(x-y)\, a_{y,j} + \sum_{x\in X} a^*_{x,i}\phi^X_{ij}(x)a_{x,j} \\ &\quad + \sum_{(x,y)\in X^2} a^*_{x,i}a_{x,i}\, W^X(x-y)\, a^*_{y,j}a_{y,j} - \mu\, \mathfrak{N}^X\,. \end{aligned}$$

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In order to describe infinite systems of interacting fermions one takes the thermodynamic limit of a sequence of finite systems e.g. on cubes $\Lambda_k := \{-k, \ldots, k\}^d \subset \mathbb{Z}^d$, $k \in \mathbb{N}$.

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We consider a sequence of Hamiltonians that are sums of local terms,

$$H_0^{\Lambda_k} = \sum_{X \subset \Lambda_k} \Phi^{\Lambda_k}(X)\,,$$

where $\Phi^{\Lambda_k}(X) \in \mathcal{A}_X$ and $\|\Phi^{\Lambda_k}(X)\|$ is small if $\operatorname{diam} X$ is large.

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A family $B = \{B^{\Lambda_k}\}$ of self-adjoint operators B^{Λ_k} indexed by the domain Λ_k and possibly other parameters that is a sum of local terms,

$$B^{\Lambda_k} = \sum_{X \subset \Lambda_k} \Phi_B^{\Lambda_k}(X)$$

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$$\|B^{\Lambda_k}\| \sim |\Lambda_k| = (2k+1)^d \,.$$

Interacting fermions on the lattice

To quantify locality of SLT operators, one defines spaces $\mathcal{B}_\zeta$ of SLT operators with norm

$$\|\Phi\|_\zeta \;:=\; \sup_{k\in\mathbb{N}} \sup_{x\in\Lambda_k} \sum_{X\subset\Lambda_k,\, x\in X} \frac{\|\Phi^{\Lambda_k}(X)\|}{\zeta(\mathrm{diam}(X))} \;=:\; \sup_{k\in\mathbb{N}} \|\Phi\|_{\zeta,\Lambda_k}\,,$$

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Definition

One says that an SLT operator in $\mathcal{B}_\zeta$ has a thermodynamic limit , if for all $M \in \mathbb{N}$ and $\delta > 0$ there exists $K \geq M$ such that for all $l, k \geq K$

$$\left\| \Phi^{\Lambda_l} - \Phi^{\Lambda_k} \right\|_{\zeta,\Lambda_M} \ \leq \ \delta \, .$$

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We say that an SLT operator in $\mathcal{B}_\zeta$ has a rapid thermodynamic limit with exponent $\gamma \in (0,1)$, if there exist $\lambda, C > 0$ such that for all $M \in \mathbb{N}$ and for all $l, k \geq M + \lambda M^\gamma$

$$\left\| \Phi^{\Lambda_l} - \Phi^{\Lambda_k} \right\|_{\zeta,\Lambda_M} \leq C\,\zeta(M^\gamma) =: C\,\zeta_\gamma(M)\,.$$

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$$\left\|\Phi^{\Lambda_l} - \Phi^{\Lambda_k}\right\|_{\zeta,\Lambda_M} \leq C\,\zeta(M^\gamma) =: C\,\zeta_\gamma(M)\,.$$

However, there is no limiting Hamiltonian for the infinite system!

Interacting fermions on the lattice

Since for $Y \subset X$ we have $\mathcal{A}_Y \subset \mathcal{A}_X$, one can define the algebra of local observarbles as

$$\mathcal{A}_{\mathrm{loc}} := \bigcup_{X \subset \mathbb{Z}^d,\, |X| < \infty} \mathcal{A}_X \,.$$

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In order to regain control on the localisation properties of elements of $\mathcal{A}$, one defines sub-algebras $\mathcal{D}_\zeta \subset \mathcal{A}$ with norm

$$\|B\|_\zeta := \|B\| + \sup_{k \in \mathbb{N}} \left(\frac{\| (1 - \mathbb{E}_{\Lambda_k}) (B) \|}{\zeta(k)} \right) < \infty \,,$$

where $\zeta : [0, \infty) \to (0, \infty)$ is again a rapidly decaying function and $\mathbb{E}_{\Lambda_k} : \mathcal{A} \to \mathcal{A}_{\Lambda_k}$ denotes the conditional expectation.

Interacting fermions on the lattice

Proposition

Let $H_0 \in \mathcal{B}_\zeta$ have a thermodynamic limit.

Then for any $B \in \mathcal{A}_{\mathrm{loc}}$ the limit

$$\mathfrak{U}_t(B) := \lim_{k\to\infty} \mathrm{e}^{\mathrm{i}H_0^{\Lambda_k} t}\, B\, \mathrm{e}^{-\mathrm{i}H_0^{\Lambda_k} t} \in \mathcal{A}$$

exists and defines a one-parameter family $t \mapsto \mathfrak{U}_t$ of automorphisms of the algebra $\mathcal{A}$ with densely defined generator $\mathcal{L}_{H_0} : D(\mathcal{L}_{H_0}) \to \mathcal{A}$.

Interacting fermions on the lattice

Proposition

Let $H_0 \in \mathcal{B}_\zeta$ have a thermodynamic limit.

Then for any $B \in \mathcal{A}_{\mathrm{loc}}$ the limit

$$\mathfrak{U}_t(B) := \lim_{k\to\infty} \mathrm{e}^{\mathrm{i}H_0^{\Lambda_k} t}\, B\, \mathrm{e}^{-\mathrm{i}H_0^{\Lambda_k} t} \in \mathcal{A}$$

exists and defines a one-parameter family $t \mapsto \mathfrak{U}_t$ of automorphisms of the algebra $\mathcal{A}$ with densely defined generator $\mathcal{L}_{H_0} : D(\mathcal{L}_{H_0}) \to \mathcal{A}$.

Moreover, for suitable pairs f_1, f_2 of rapidly decaying functions,

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Also the Liouvillian

$$\mathcal{L}_{H_0} : \mathcal{D}_{f_1} \to \mathcal{D}_{f_2}\,, \quad \mathcal{L}_{H_0}(B) := \lim_{k\to\infty} [H_0^{\Lambda_k}, \mathbb{E}_{\Lambda_k}(B)]$$

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If $H_0 \in \mathcal{B}_\zeta$ has a rapid thermodynamic limit with exponent $\gamma \in (0,1)$, then there exist $\lambda_1 > 0$, $\lambda_2 \in (0,1)$, and $C < \infty$, such that for all $l, k \in \mathbb{N}$ with $l \geq k$, $X \subset \Lambda_k$ and $B \in \mathcal{A}_X$

$$\begin{aligned}\left\| \left(\mathfrak{U}_t^{\Lambda_l} - \mathfrak{U}_t^{\Lambda_k}\right)(B)\right\| \;\leq\;& C\,\|B\|\,\mathrm{diam}(X)^{d+1}\,\mathrm{e}^{2C_\zeta|t-s|\|\Phi_{H_0}\|_\zeta}|t-s| \\ & \times \zeta_\gamma\left(\mathrm{dist}^{\Lambda_l}(X, \Lambda_l \setminus \Lambda_{\max\{\lceil k-\lambda_1 k^\gamma\rceil, \lceil \lambda_2\cdot k\rceil\}})\right)\end{aligned}$$

Adiabatic theorem

From now on we consider a time-dependent SLT Hamiltonian $H_0(t) \in \mathcal{B}_{\mathrm{e}^{-a\,\cdot}}$, $t \in I \subset \mathbb{R}$, possibly perturbed by a time-dependent operator $\varepsilon V(t)$, where $V(t) = V_v(t) + H_1(t)$ is the sum of an SLT operator $H_1(t)$ and a Lipschitz potential $V_v(t)$, i.e.

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Similar results as before hold for the corresponding adiabatic evolution family $\mathfrak{U}^{\eta,\varepsilon}_{t,t_0}$ generated by the time-dependent Liouvillian $\frac{1}{\eta}\mathcal{L}_{H_\varepsilon(t)}$ with adiabatic parameter $\eta > 0$, i.e.

$$\mathfrak{U}^{\eta,\varepsilon}_{t,t_0}(B) := \lim_{k\to\infty} \mathfrak{U}^{\eta,\varepsilon,\Lambda_k}_{t,t_0}(B) \in \mathcal{A}$$

Adiabatic theorem

Standard gap assumption

Assume that smallest eigenvalue $E_0^{\Lambda_k}(t)$ (ground state) of $H_0^{\Lambda_k}(t)$ is separated from the rest of the spectrum uniformly in the volume $|\Lambda_k|$,

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

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Adiabatic theorems under the "standard gap assumption" in finite volumes with error estimates that are uniform in the volume were shown by **Bachmann, De Roeck, Fraas** CMP '18, **Monaco, T.**, RMP '19 and **T.**, CMP '20.

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In **Henheik, T.** ’20 we prove an adiabatic theorem for $\mathfrak{U}_{t,t_0}$ on $\mathcal{A}$ and apply it to linear response.

Adiabatic theorem with a gap in the bulk

Motivation: Response of Chern-nontrivial systems (e.g. quantum Hall systems), where the Hamiltonian has no spectral gap due to edge states.

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for all $B \in \mathcal{A}$ and $s \in \mathbb{R}$.

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H_ρ is called the bulk Hamiltonian associated with ρ.

Adiabatic theorem with a gap in the bulk

Gap assumption in the bulk (cf. Moon, Ogata, JFA '19)

There exists $g > 0$ such that for each $t \in I$ the Liouvillian $\mathcal{L}_{H_0(t)}$ has a unique ground state ρ_t and

$$\sigma(H_{\rho_t}) \setminus \{0\} \subset [g, \infty).$$

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Adiabatic theorem

Let the Hamiltonian $H_\varepsilon(t) = H_0(t) + \varepsilon V(t)$ satisfy the previous assumptions and denote by $\mathfrak{U}^{\varepsilon,\eta}_{t,t_0}$ the Heisenberg time-evolution it generates on $\mathcal{A}$.

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has the following properties:

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has the following properties:

(1) It almost intertwines the time evolution: For any $n \in \mathbb{N}$ and any $f \in \mathcal{S}$, there exists a constant C_n such that for any $t \in I$ and $B \in \mathcal{D}_f$

$$\left| \left(\Pi^{\varepsilon,\eta}_{t_0} \circ \mathfrak{U}^{\varepsilon,\eta}_{t,t_0} - \Pi^{\varepsilon,\eta}_t \right) (B) \right| \leq C_n \, \frac{\varepsilon^{n+1} + \eta^{n+1}}{\eta^{d+1}} \left(1 + |t - t_0|^{d+1} \right) \|B\|_f .$$

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(3) It is stationary whenever the Hamiltonian is stationary: if H_ε is constant on an interval $J \subset I$ then $\Pi^{\varepsilon,\eta}_t = \Pi^{\varepsilon,0}_t$ is constant for $t \in J$.

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(4) $\Pi^{\varepsilon,0}_t$ has an explicit asymptotic expansion in powers of ε.

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has the following properties:

(5) It equals the ground state of H_0 whenever the perturbation vanishes and the Hamiltonian is stationary: if for some $t \in I$ all time-derivatives of H_ε vanish at time t and $V(t) = 0$, then $\Pi^{\varepsilon,\eta}_t = \Pi^{\varepsilon,0}_t = \rho_t$.

Remark on time-scales

For $\varepsilon \neq 0$, the right hand side of

$$\begin{aligned}\left|\left(\Pi_{t_0}^{\varepsilon,\eta} \circ \mathfrak{U}_{t,t_0}^{\varepsilon,\eta} - \Pi_t^{\varepsilon,\eta}\right)(B)\right| \\ \leq \; C_n \, \frac{\varepsilon^{n+1} + \eta^{n+1}}{\eta^{d+1}} \, \left(1 + |t - t_0|^{d+1}\right) \|B\|_f\end{aligned}$$

shows that the admissible adiabatic time scales η are coupled to the strength ε of the perturbation:

The adiabatic parameter η needs to be small, but not too small. The adiabatic switching must occur on time-scales that are fast compared to the life-time of the NEASS, i.e. $\eta \gtrsim \varepsilon^m$ for some $m \in \mathbb{N}$.

Remark on finite domains

Under an additional assumption on the rate of convergence in

$$\rho^{\Lambda_k} \to \rho$$

we show that a similar adiabatic theorem holds also for finite systems up to an additional error term that decays faster than any inverse polynomial in the system size.

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There exists $\lambda > 0$ such that for any $n \in \mathbb{N}$ there exists a constant C_n and for any compact $K \subset I$ and $m \in \mathbb{N}$ there exists a constant $\tilde{C}_{n,m,K}$ such that for all $k \in \mathbb{N}$, all finite $X \subset \Lambda_k$, all $B \in \mathcal{A}_X$, and all $t, t_0 \in K$

$$\begin{aligned} &\left| \left(\Pi_{t_0}^{\varepsilon,\eta,\Lambda_k} \circ \mathfrak{U}_{t,t_0}^{\varepsilon,\eta,\Lambda_k} - \Pi_t^{\varepsilon,\eta,\Lambda_k} \right)(B) \right| \\ &\qquad \leq \; C_n \, \frac{\varepsilon^{n+1} + \eta^{n+1}}{\eta^{d+1}} \, \left(1 + |t - t_0|^{d+1} \right) \, \|B\| \, |X|^2 \\ &\qquad\quad + \; \tilde{C}_{n,m,K} \, \left(1 + \eta \, \mathrm{dist}(X, \Gamma \setminus \Lambda_{\lfloor k - \lambda k^\gamma \rfloor}) \right)^{-m} \|B\| \, \mathrm{diam}(X)^{2d}. \end{aligned}$$

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In finite volume Λ, where ρ is the ground state projection, the construction of the (stationary) NEASS proceeds as follows:

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$$[H, \Pi] \;=\; \left[H_0 + \varepsilon V, \mathrm{e}^{\mathrm{i}\varepsilon S}\rho\,\mathrm{e}^{-\mathrm{i}\varepsilon S}\right]$$

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We thus need to choose A_1 such that

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\left[\mathcal{L}_{H_0}(A_1) - \mathrm{i} V, \rho \right] \stackrel{!}{=} 0
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Assuming a spectral gap for H_0, **Bachmann, Michalakis, Nachtergaele, Sims**, CMP '12 (based on **Hastings, Wen**, PRB '05) constructed a linear map

$$\mathcal{I}^{\Lambda}_{H_0,g} : \mathcal{A}_\Lambda \to \mathcal{A}_\Lambda$$

that maps SLT operators to SLT operators and satisfies

$$\mathcal{I}^{\Lambda}_{H_0,g}|_{\mathcal{A}^{\mathrm{OD}}_\Lambda} = \mathrm{i}\, \mathcal{L}^{-1}_{H_0}|_{\mathcal{A}^{\mathrm{OD}}_\Lambda} \,.$$

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Thus, for all $A \in \mathcal{A}_\Lambda$,

$$\left[\mathcal{L}_{H_0} \circ \mathcal{I}^{\Lambda}_{H_0,g}(A) - \mathrm{i}A, \rho\right] = 0$$

and one can choose $A_1 = \mathcal{I}^{\Lambda}_{H_0,g}(V)$.

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Based on techniques of **Moon, Ogata**, *JFA* '19 we show that

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exists as a bounded operator from $\mathcal{D}_{f_1}$ to $\mathcal{D}_{f_2}$ and satisfies:

Lemma

Let H_0 have a gap in the bulk.
Then for all $A \in \mathcal{A}$ with $\mathcal{I}_{H_0,g}(A) \in D(\mathcal{L}_{H_0})$ and all $B \in D(\mathcal{L}_{H_0})$

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Let H_0 have a gap in the bulk.
Then for all $A \in \mathcal{A}$ with $\mathcal{I}_{H_0,g}(A) \in D(\mathcal{L}_{H_0})$ and all $B \in D(\mathcal{L}_{H_0})$

$$\rho\big(\big[\mathcal{L}_{H_0} \circ \mathcal{I}_{H_0,g}(A) - \mathrm{i}A, B\big]\big) = 0\,.$$

Problem: $V \notin \mathcal{A}$.

Elements of the proof: the local inverse of the Liouvillian

Based on techniques of **Moon, Ogata**, *JFA* '19 we show that

$$\mathcal{I}_{H_0,g} := \lim_{k\to\infty} \mathcal{I}_{H_0,g}^{\Lambda_k}$$

exists as a bounded operator from $\mathcal{D}_{f_1}$ to $\mathcal{D}_{f_2}$ and satisfies:

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Let H_0 have a gap in the bulk.
Then for all $A \in \mathcal{A}$ with $\mathcal{I}_{H_0,g}(A) \in D(\mathcal{L}_{H_0})$ and all $B \in D(\mathcal{L}_{H_0})$

$$\rho\big(\big[\mathcal{L}_{H_0} \circ \mathcal{I}_{H_0,g}(A) - \mathrm{i}A, B\big]\big) = 0\,.$$

Problem: $V \notin \mathcal{A}$.
Solution: Take the thermodynamic limit for H_0 and the perturbation V independently.

Concluding remarks

- Proving uniqueness of the ground state ρ of $\mathcal{L}_{H_0}$ and “fast convergence” of $\rho^{\Lambda_k} \to \rho$, e.g.

$$|(\rho - \rho^{\Lambda})(B)| \leq C_n \|B\| \mathrm{dist}(X, \partial\Lambda)^{-n}$$

for all $B \in \mathcal{A}_X$, are difficult problems that have not yet been achieved for interacting fermionic systems.

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  For weakly interacting spin systems such a result has been shown by **Yarotzky**, JSP '05.

- A similar justification of linear response for systems with mobility gap instead of spectral gap is a difficult open problem even for non-interacting systems.

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Thanks for your attention!

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