Transport for the 1D Schrödinger equation via quasi-free systems

(Collaboration with V. Jaksic)

L. Bruneau

Univ. Cergy-Pontoise

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  Localization if $\sup_t \langle \psi_t, \langle X \rangle^n \psi_t \rangle \leq C_n$ and transport if $\langle \psi_t, \langle X \rangle^n \psi_t \rangle \simeq C_n t^{n\beta(n)}$ with $\beta(n) > 0$ (transport exponent).

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- Spectral: $\mathrm{sp}_{\mathrm{pp}}(H)$ is associated to the notion of localization and $\mathrm{sp}_{\mathrm{ac}}(H)$ to the one of transport.

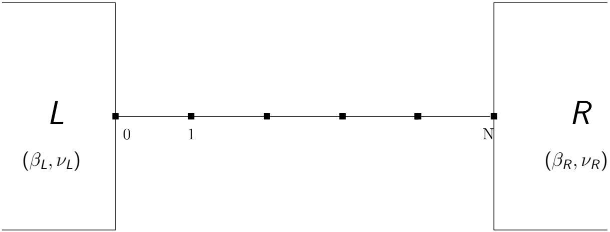
Between these 2 notions there are links but no equivalence:

- $E \in \mathrm{sp}_{\mathrm{pp}}(H)$ and ψ^E an eigenfunction, then $\langle \psi_t^E, \langle X\rangle^n \psi_t^E\rangle = C$: dynamical loc.
- dynamical loc. $\Rightarrow$ pp spectrum (RAGE theorem).
- $\psi \in \mathcal{H}_{\mathrm{ac}}$: $\frac{1}{T}\int_0^T \langle \psi_t, \langle X\rangle^n \psi_t\rangle \mathrm{d}t \ge C_n T^{n/d}$ [Guarneri '93].
- pp spectrum $\not\Rightarrow$ dynamical loc., see e.g. [GKT,JSS,DJLS].

Huge amount of litterature on the subject.

Approach via quantum statistical mechanics

Consider the case $\ell^2(\mathbb{Z})$. We couple a finite sample to 2 reservoirs.



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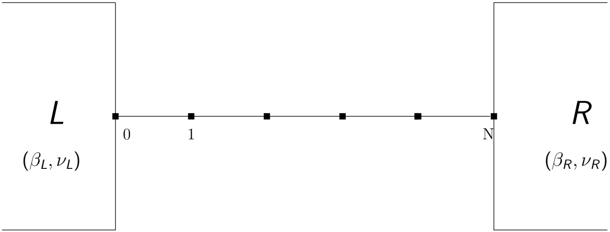

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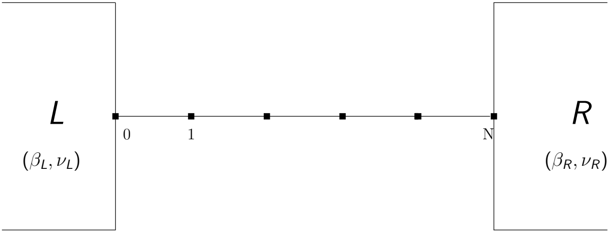

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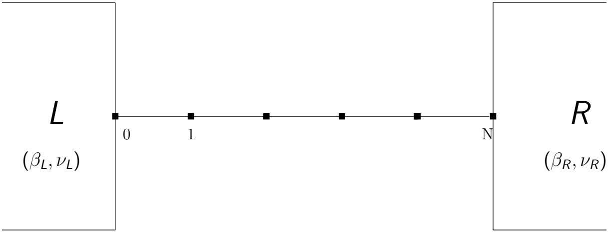

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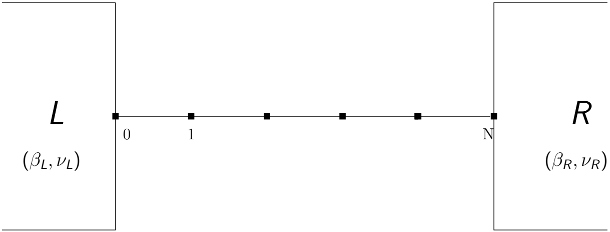

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1. We let the system relax to the NESS ω_+.
2. If J_L is the observable "current out of L", we calculate $\omega_+(J_L) =: \langle J_L \rangle_+^N$ (the sample has size N).
3. We study the behaviour of $\langle J_L \rangle_+^N$ as $N \to \infty$ according to the properties of V (or of $-\Delta + V$): does it go to 0? at which rate? is there a non trivial (positive) limit?

Quasi-free systems

Independent electrons approximation: free fermi gas with a 1 particle space of the form

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1 particle hamiltonian: $h = h_0 + w$ where

$$h_0 = h_L \oplus (-\Delta + V)_D \oplus h_R, \quad w = |\delta_L\rangle\langle\delta_0| + |\delta_0\rangle\langle\delta_L| + |\delta_R\rangle\langle\delta_N| + |\delta_N\rangle\langle\delta_R|.$$

$(\mathfrak{h}_{L/R}, h_{L/R})$: "free" reservoirs with good ergodic properties: we assume that the spectral measures $\mu_{L/R}$ of $h_{L/R}$ for $\delta_{L/R}$ are purely a.c.

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$$\mathfrak{h}_{L/R} = L^2(\mathbb{R}, \mathrm{d}\mu_{L/R}(E)), \quad h_{L/R} = \text{mult par } E, \quad \delta_{L/R} = 1.$$

Examples: free Laplacian on half-line , full line , Bethe lattice , 1/2-space,...

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$$H = \mathrm{d}\Gamma(h) = H_0 + a^*(\delta_L)a(\delta_0) + a^*(\delta_0)a(\delta_L) + a^*(\delta_R)a(\delta_N) + a^*(\delta_N)a(\delta_R).$$

For any $A \in \mathcal{O}$, $\tau_t(A) := \mathrm{e}^{itH} A \mathrm{e}^{-itH}$. In particular, for $f \in \mathfrak{h}$ one has $\tau_t(a^\#(f)) = a^\#(\mathrm{e}^{ith} f)$.

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Initial state of the system: quasi-free state ω_0 associated to the density matrix

$$T = (1 + \mathrm{e}^{\beta(h_L - \nu_L)})^{-1} \oplus \rho_S \oplus (1 + \mathrm{e}^{\beta(h_R - \nu_R)})^{-1},$$

i.e. ω_0 is such that

$$\omega_0(a^*(g_n) \cdots a^*(g_1) a(f_1) \cdots a(f_m)) = \delta_{nm} \mathrm{det}(\langle f_i, T g_j \rangle)_{i,j}.$$

The current observable

The number of fermions in reservoir L is $N_L = \mathrm{d}\Gamma(\mathbb{1}_L)$ where $\mathbb{1}_L$ is the projection onto $h_L \simeq h_L \oplus 0 \oplus 0$. The observable which describes the flux of particles out of L is therefore

$$J_L := -\frac{\mathrm{d}}{\mathrm{d}t}\tau_t(N_L)\Big|_{t=0} = -i[H, N_L] = a^*(i\delta_L)a(\delta_0) + a^*(\delta_0)a(i\delta_L).$$

Remark: $J_L = \mathrm{d}\Gamma(j_L)$ where $j_L = i|\delta_L\rangle\langle\delta_0| - i|\delta_0\rangle\langle\delta_L| = -i[h, \mathbb{1}_L]$.

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We are interested in

$$\langle J_L\rangle_+^N := \lim_{T\to+\infty} \frac{1}{T}\int_0^T \omega\circ\tau_t(J_L)\mathrm{d}t = \omega_+(J_L),$$

where $\omega_+ = w* - \lim \frac{1}{T}\int_0^T \omega_0\circ\tau^t$ is the NESS of the system (if it exists), and in particular to the large N behaviour of $\langle J_L\rangle_+^N$.

NESS and 1 paticle scattering

(Hyp) $\quad \mathrm{sp}_{\mathrm{sc}}(h) = \emptyset$

Theorem (AJPP '07)

1) There is a unique NESS ω_+.
2) The wave operators $W_\pm := s - \lim_{t\to\pm\infty} \mathrm{e}^{-ith_0}\mathrm{e}^{ith}\mathbb{1}_{\mathrm{ac}}(h)$ *exist and are complete. The restriction of* ω_+ *to* $CAR(\mathfrak{h}_{\mathrm{ac}}(h))$ *is the quasi-free state with density matrix* $W_-^* T W_-$.
3) If c *is trace class on* $\mathfrak{h}$*, then* $\omega_+(\mathrm{d}\Gamma(c)) = \mathrm{Tr}(T_+ c)$ *where*

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Corollary: with $c = j_L$ we get

$$\langle J_L\rangle_+^N = 2\mathrm{Im}\langle W_-\delta_L, TW_-\delta_0\rangle.$$

Reformulation of the current

Lemma

$$\langle J_L\rangle_+^N = 2\pi\int_{\mathbb{R}} |G(0,N;E+i0)|^2 \left[\frac{1}{1+\mathrm{e}^{\beta(E-\nu_L)}} - \frac{1}{1+\mathrm{e}^{\beta(E-\nu_R)}}\right] \frac{\mathrm{d}\mu_L}{\mathrm{d}E}\frac{\mathrm{d}\mu_R}{\mathrm{d}E}\mathrm{d}E.$$

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Remark 2: If $\nu_L \geq \nu_R$ we indeed have $\langle J_L\rangle_+^N \geq 0$.

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Proof:

1) Explicit calculation of the wave operators: if $f = f_L \oplus f_S \oplus f_R$ one has

$$W_- f = f_L^- \oplus 0 \oplus f_R^-, \quad f_{L/R}^-(E) = f_{L/R}(E) - \langle\delta_{0/N}, (h-E+i0)^{-1} f\rangle.$$

Reformulation of the current

2) Insert this in $\langle J_L\rangle_+^N = 2\mathrm{Im}\langle W_-\delta_L, TW_-\delta_0\rangle$:

$$\begin{aligned}\langle J_L\rangle_+^N \;=\;& 2\mathrm{Im}\int \big(G(L,0;E+i0)G(0,0;E-i0) - G(0,L;E-i0)\big)\\ &\qquad\times\frac{1}{1+\mathrm{e}^{\beta(E-\nu_L)}}\mathrm{d}\mu_L(E)\\ &+2\mathrm{Im}\int G(L,N;E+i0)G(N,0;E-i0)\frac{1}{1+\mathrm{e}^{\beta(E-\nu_R)}}\mathrm{d}\mu_R(E).\end{aligned}$$

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3) At equilibrium, i.e. $\nu_L = \nu_R$, $\langle J_L\rangle_+^N = 0$.

$$\begin{aligned}\Rightarrow \quad \langle J_L\rangle_+^N &= 2\mathrm{Im}\int G(L,N;E+i0)G(N,0;E-i0) \\ &\qquad \times \left[\frac{1}{1+\mathrm{e}^{\beta(E-\nu_R)}} - \frac{1}{1+\mathrm{e}^{\beta(E-\nu_L)}}\right]\mathrm{d}\mu_R(E).\end{aligned}$$

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4) Resolvent identity gives

$$G(L,N;E+i0) = -\langle\delta_L,(h_0 - E - i0)^{-1}\delta_L\rangle \times G(0,N;E+i0),$$

and one uses $\mathrm{Im}\langle\delta_L,(h_0-E-i0)^{-1}\delta_L\rangle = \pi\frac{\mathrm{d}\mu_L}{\mathrm{d}E}$.

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2) There is transport at energy E if $\liminf_{N\to\infty} \langle J_L \rangle_+^N(E) > 0$, *where*

$$\langle J_L \rangle_+^N(E) = 2\pi |G(0,N;E+i0)|^2 \left[\frac{1}{1+\mathrm{e}^{\beta(E-\nu_L)}} - \frac{1}{1+\mathrm{e}^{\beta(E-\nu_R)}} \right] \frac{\mathrm{d}\mu_L}{\mathrm{d}E} \frac{\mathrm{d}\mu_R}{\mathrm{d}E}$$

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Idea: L very large, i.e. $\mathrm{sp}(h_L) \simeq \mathbb{R}$, and R only has energies close to E, i.e. $\mathrm{sp}(h_R) \simeq [E-\epsilon, E+\epsilon]$, then $\langle J_L\rangle_+^N \simeq 2\epsilon \langle J_L\rangle_+^N(E)$.

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Proposition

Whether there is transport or no at energy E does not depend on the boundary condition.
If moreover $\lim\limits_{N\to\infty} \langle J_L\rangle_+^N(E) = 0$, then the convergence speed does not depend on the boundary condition.

Proof: repeated use of the resolvent identity.

A.c. Spectrum = Transport

Theorem

1) For Lebesgue almost all $E \in \mathrm{sp}_{\mathrm{ac}}(h_\infty) \cap \mathrm{sp}(h_L) \cap \mathrm{sp}(h_R)$ *there is transport at energy* E.
2) If $\lambda\left(\mathrm{sp}_{\mathrm{ac}}(h_\infty) \cap \mathrm{sp}(h_L) \cap \mathrm{sp}(h_R)\right) > 0$ *there is transport.*

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Remark 1: Changing the boundary condition induces a rank 1 perturbation on h_∞ and hence does not change its a.c. spectrum.
Remark 2: In the 2nd theorem, the nature of the singular spectrum does not matter.

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If the spectrum of h_∞ is pure point one expects a better localization, e.g. $\lim \langle J_L \rangle_+^N(E) = 0$ instead of $\liminf \langle J_L \rangle_+^N(E) = 0$.

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Examples where the spectrum of h_∞^0 is pure point but that of h_∞^α is purely s.c. for $\alpha \neq 0$, e.g. [Simon-Wolff '86].
[Gordon '94]: one can not have p.p. spectrum for all α's.
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P.p. Spectrum (I)

If the spectrum of h_∞ is pure point one expects a better localization, e.g. $\lim \langle J_L \rangle_+^N(E) = 0$ instead of $\liminf \langle J_L \rangle_+^N(E) = 0$.

Problem: $\mathrm{sp}(h_\infty) = \mathrm{sp}_{\mathrm{pp}}(h_\infty)$ is not sufficient!
Why?: boundary condition has no influence on transport but the singular spectrum is very sensitive even to rank 1 perturbations.

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Conclusion: one has to rule out s.c. spectrum for almost-all α.

Rank 1 perturbations

Let $F_\alpha(z) := \langle \delta_0, (h_\infty^\alpha - z)^{-1}\delta_0\rangle$, $G(x) := \lim_{y\downarrow 0} \frac{1}{y}\mathrm{Im} F_0(x+iy)$.

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Facts: 1) $F_\alpha(x) = \lim_{y\downarrow 0} F_\alpha(x+iy)$ exists, is finite and non-zero for Lebesgue almost all x.

2) $G(x) = \infty$ for μ_0 almost all x where μ_0 is the spectral measure of h_∞^0 for δ_0, i.e. s.t. $F_0(z) = \int \frac{\mathrm{d}\mu_0(t)}{t-z}$.

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For $\alpha \neq 0$, let

$$
\begin{aligned}
T_\alpha &= \{x\in\mathbb{R} \; : \; F_0(x) = -\alpha^{-1},\ G(x) < \infty\},\\
S_\alpha &= \{x\in\mathbb{R} \; : \; F_0(x) = -\alpha^{-1},\ G(x) = \infty\},\\
L &= \{x\in\mathbb{R} \; : \; \mathrm{Im} F_0(x) > 0\}.
\end{aligned}
$$

Rank 1 perturbations and p.p. spectrum (II)

Theorem (Aronszajn-Donoghue)

1) T_α is the set of e.v. of h_∞^α.
2) $\mu_{\rm sc}^\alpha$ is concentrated on S_α.
3) For all α, L is the essential support of the a.c. spectrum of h_∞^α.

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Let $B \subset \mathbb{R}$ be a borel set. The following are equivalent
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Theorem

Let $I \subset \mathbb{R}$ s.t. $G(E) < \infty$ for $E \in I$, then $\lim_{N\to\infty} \langle J_L \rangle_+^N(E) = 0$.

Lyapunov exponents

Let $T_E(n)$ denote the transfer matrix at energy E, i.e.

$$T_n(E) = \begin{pmatrix} E - V(n-1) & -1 \\ 1 & 0 \end{pmatrix} \times \cdots \times \begin{pmatrix} E - V(0) & -1 \\ 1 & 0 \end{pmatrix}.$$

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The Lyapunov exponent is defined, when it exists, by

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Theorem

Let E such that $\gamma(E) > 0$, then

$$\lim_{N\to\infty} \frac{1}{N} \log(\langle J_L \rangle_+^N(E) + \langle J_L \rangle_+^{N+1}(E)) = -2\gamma(E).$$

Main arguments of the proof

1. Rewrite $G(x, y; z) = \langle \delta_x, (h - z)^{-1} \delta_y \rangle$ for $x, y = 0, N$ in terms of $G_S(x, y; z) = \langle \delta_x, (h_S - z)^{-1} \delta_y \rangle$ where $h_S = -\Delta + V$ sur $\ell^2([0, N])$.

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2. Express $G_S(x,y;E)$ in terms of generalized eigenfunctions of h_∞ (and hence in terms of $T_E(N)$) and study their behaviour.
3. Use the independence w.r.t. the boundary condition.
4. Use results of [Last-Simon '99] which relate the nature of the spectrum to the behaviour of $T_E(n)$:
   - $S = \{E, \ \liminf \| T_E(n,0)\| < \infty\}$ supports the a.c. spectrum of h_∞,
   - $S' = \{E, \ \liminf \frac{1}{N}\sum_{n=1}^N \| T_E(n,0)\|^2 < \infty\}$ is an essential support of the a.c. spectrum of h_∞ and has zero measure with repsect to the singular part part of the spectral measure.