Conductances, a.c. spectrum and periodic approximants of 1D systems

(Collaboration with V. Jakšić, Y. Last and C.-A. Pillet)

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Plan

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Connection between transport in non-equilibrium quantum statistical mechanics and spectral theory (of Jacobi matrices).

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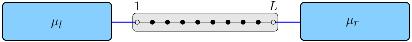

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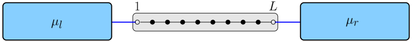

Dynamical characterization of spectral types (ac, sc, pp):

1. take $h = -\Delta + v$ on $\mathbb{Z}_+$,
2. restrict to $\{1, \ldots, L\}$,
3. analyze the associated conductance as $L \to \infty$.

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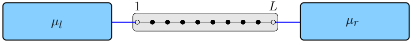

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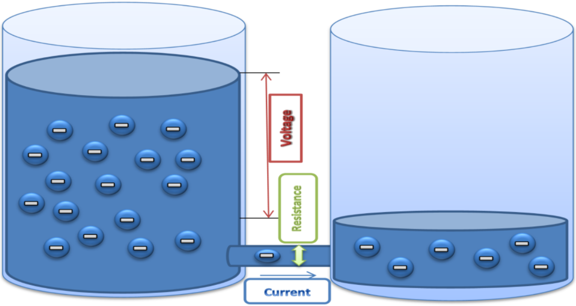
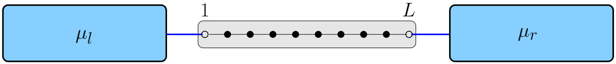
Physics literature: transport theory of 1D systems goes back to 70's (Anderson, Thouless, Landauer,...)

Math literature: mostly absent until the last 10 years and the rigorous derivation of Landauer [Aschbacher-Jakšić-Pautrat-Pillet '07, Nenciu '07] and Thouless [B-Jakšić-Last-Pillet '15] formulas from first principles.

An analogy





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Setup: one electron data

A sample $\mathcal{S}$ coupled to 2 electronic reservoirs $\mathcal{R}_{l/r}$ described by free fermi gases at equilibrium (at zero temperature and chemical potential $\mu_{l/r}$) and in the independent electron approximation.

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Reservoirs: the one electron data are $(\mathfrak{h}_{l/r}, h_{l/r}, \psi_{l/r})$ where $\psi_{l/r}$ are cyclic vectors for $h_{l/r}$. In the spectral representation,

$$\mathfrak{h}_{l/r} = L^2(\mathbb{R}, \mathrm{d}\nu_{l/r}(E)), \quad h_{l/r} = \text{mult by } E, \quad \psi_{l/r}(E) \equiv 1,$$

where $\nu_{l/r}$ is the spectral measure for $h_{l/r}$ and $\psi_{l/r}$.

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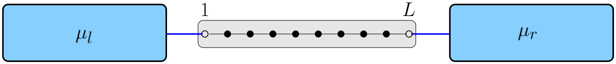
Coupled one electron system: $\mathfrak{h} = \mathfrak{h}_l \oplus \mathfrak{h}_L \oplus \mathfrak{h}_r$ and $h_{\kappa,L} = h_{0,L} + \kappa h_T$ where

$$h_{0,L} = h_l \oplus h_L \oplus h_r, \quad h_T = |\psi_l\rangle\langle\delta_1| + |\delta_1\rangle\langle\psi_l| + |\psi_r\rangle\langle\delta_L| + |\delta_L\rangle\langle\psi_r|.$$



Setup: many electrons

The full system is the corresponding Free Fermi gas with reservoirs initially at equilibrium:

- Hilbert space: the fermionic Fock space $\Gamma_-(\mathfrak{h}) = \oplus_{n=0}^{\infty} \wedge^n \mathfrak{h}$.
- Hamiltonian: the second quantized operator $H = \mathrm{d}\Gamma(h_{\kappa,L})$, i.e.

$$H\, f_1 \wedge \cdots \wedge f_n = \sum_{j=1}^{n} f_1 \wedge \cdots \wedge h_{\kappa,L} f_j \wedge \cdots \wedge f_n .$$

- Initial state: quasi-free state ω_0 generated by the density operator $T = T_l \oplus T_L \oplus T_r$ where $T_{l/r} = \mathbb{1}_{(-\infty,\mu_{l/r}]}(h_{l/r})$.

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- Charge current observable:

$$\mathcal{J} := -i[H, N_r] = \kappa(a^*(i\psi_r)a(\delta_L) + a^*(\delta_L)a(i\psi_r))$$

where $N_r = \mathrm{d}\Gamma(\mathbb{1}_r)$ is the number of fermions in reservoir $\mathcal{R}_r$ ($\mathbb{1}_r$ is the projection onto $h_r \simeq 0 \oplus 0 \oplus h_r$).

Landauer-Büttiker formula

The steady state expectation value of the charge current observable is given by the Landauer-Büttiker formula [Landauer '70], proven by [AJPP '07, N'07] provided $\mathrm{sp}_{\mathrm{sc}}(h_{\kappa,L}) = \emptyset$.

$$\omega_+(\mathcal{J}) := \lim_{T\to+\infty} \frac{1}{T}\int_0^T \omega_0\left(\mathrm{e}^{itH}\mathcal{J}\mathrm{e}^{-itH}\right)\mathrm{d}t \;=\; \frac{1}{2\pi}\int_{\mu_l}^{\mu_r} \mathcal{T}_L(E)\mathrm{d}E,$$

where $\mathcal{T}_L(E)$ is the transmission probability at energy E for the pair $(h_{\kappa,L}, h_{0,L})$.

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where $\mathcal{T}_L(E)$ is the transmission probability at energy E for the pair $(h_{\kappa,L}, h_{0,L})$. Stationary scattering theory gives

$$\mathcal{T}_L(E) = 4\pi^2\kappa^4 |\langle\delta_1, (h_{\kappa,L} - E - i0)^{-1}\delta_L\rangle|^2 \frac{\mathrm{d}\nu_{l,\mathrm{ac}}}{\mathrm{d}E}(E)\frac{\mathrm{d}\nu_{r,\mathrm{ac}}}{\mathrm{d}E}(E).$$

Remark 1: Only energies in ac spectra of reservoirs contribute.
Remark 2: $\mu_{l/r}$ have a "double role": induce the current and fix the energy window.

The Landauer conductance associated to the energy window $I = (\mu_l, \mu_r)$ is $G_{LB}(L, I) = \frac{\omega_+(\mathcal{J})}{\mu_r - \mu_l}$.

Thouless formula

A particular choice of reservoirs: so that $h_{\kappa,L} = h_{\mathrm{per},L}$ is the periodic extension of the sample, i.e. the L-periodic Schrödinger on $\ell^2(\mathbb{Z})$ whose restriction to $\{1,\ldots,L\}$ is h_L.

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It amounts to take for the left, resp. right, reservoir the restriction of $h_{\mathrm{per},L}$ to $\ell^2((-\infty,0])$, resp. $\ell^2([L+1,\infty))$, with Dirichlet B.C. and $\psi_{l/r} = \delta_{0/L+1}$. The corresponding conductance $G_{Th}(L,I)$ is called Thouless conductance.

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Transport is then reflectionless: $\mathcal{T}_L(E) = 1$ if $E \in \mathrm{sp}(h_{\mathrm{per},L})$ and 0 otherwise. The Landauer-Büttiker formula thus gives

$$G_{Th}(L,I) = \frac{1}{2\pi}\frac{|\mathrm{sp}(h_{\mathrm{per},L}) \cap I|}{|I|}.$$

Remark: This is not the original definition as given by Edwards and Thouless ('72) but it amounts to it.

Plan

Formulation of the problem

Object of interest: $h = -\Delta + v$ on $\ell^2(\mathbb{Z}_+)$.

Goal: dynamical characterization of spectral types of h. Focus on ac spectrum: should be the set of energies at which the system exhibits transport, i.e.

Mathematical characterization of conducting regime

$\Updownarrow$?

Physical characterization of conducting regime

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Physical characterization of conducting regime

Definition of transport:

1. Restrict h to $\{1, \ldots, L\}$
2. Large L behavior of $G_\#(L, l)$, $\# = LB$ or Th. Does it vanish or not?

Main result

Theorem (B.-Jakšić-Last-Pillet '16)

For any potential v and any open interval I, $\# = LB$ or Th,

$$\mathrm{sp}_{\mathrm{ac}}(-\Delta+v)\cap I = \emptyset \iff \limsup_{L\to\infty} G_\#(L,I) = 0 \iff \liminf_{L\to\infty} G_\#(L,I) = 0$$

This gives a sharp characterization of ac spectrum:

- no ac spectrum in I $\Rightarrow$ corresponding conductances vansih.
- ac spectrum in I $\Rightarrow$ conductances bounded away from zero.

Mathematical characterization of conducting regime

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Physical characterization of conducting regime

Remark: For the Landauer conductance one needs to assume that the reservoirs are s.t. $\mathrm{sp}_{\mathrm{ac}}(-\Delta+v) \subset \mathrm{sp}_{\mathrm{ac}}(h_{l/r})$, transparency condition.

Periodic approximants

Denote $h^+_{\mathrm{per},L}$ the L-periodic Schrödinger on $\ell^2(\mathbb{Z}_+)$ whose restriction to $\{1,\ldots,L\}$ coincides with $h=-\Delta+v$. Then $h^+_{\mathrm{per},L} \overset{str.\,res.}{\longrightarrow} h$ (periodic approximants). By general principles the spectrum can not suddenly expand: if $\lambda \in \mathrm{sp}(h)$ there exists $\lambda_L \in \mathrm{sp}(h^+_{\mathrm{per},L})$ s.t. $\lambda_L \to \lambda$.

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$G_{Th}(L,I)=\frac{1}{2\pi|I|}|\mathrm{sp}(h_{\mathrm{per},L})\cap I|$ and $|\mathrm{sp}(h_{\mathrm{per},L})\cap I| = |\mathrm{sp}(h^+_{\mathrm{per},L})\cap I|$ (the spectra differ by a finite number of simple eigenvalues). The previous theorem means

$$\mathrm{sp}_{\mathrm{ac}}(h)\cap I=\emptyset \Leftrightarrow \limsup_{L\to\infty}|\mathrm{sp}(h^+_{\mathrm{per},L})\cap I|=0 \Leftrightarrow \liminf_{L\to\infty}|\mathrm{sp}(h^+_{\mathrm{per},L})\cap I|=0$$

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We actually have the estimate

$$\limsup_{L\to\infty}|\mathrm{sp}(h^+_{\mathrm{per},L})\cap I|\le C|\mathrm{sp}_{\mathrm{ac}}(h)\cap I|^{1/5},\qquad C\simeq 16,5.$$

In some sense the spectrum can not suddenly contract neither.

Main tool: transfer matrices

$$T(L,E) = \begin{bmatrix} v(L)-E & -1 \\ 1 & 0 \end{bmatrix} \times \cdots \times \begin{bmatrix} v(1)-E & -1 \\ 1 & 0 \end{bmatrix}.$$

u satisfies $(-\Delta + v)u = Eu$ iff $\begin{bmatrix} u(L+1) \\ u(L) \end{bmatrix} = T(L,E) \begin{bmatrix} u(1) \\ u(0) \end{bmatrix}$.

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Theorem (B.-Jakšić-Last-Pillet '16)

For any sequence $L_k \to \infty$, t.f.a.e.

1. $\mathrm{sp}_{\mathrm{ac}}(-\Delta + v) \cap I = \emptyset$.
2. $\lim G_{LB}(L_k, I) = 0$.
3. $\lim G_{Th}(L_k, I) = 0$.
4. $\lim \int_I \| T(L_k, E)\|^{-2} \mathrm{d}E = 0$.

We prove separately the equivalence between each of 1., 2., 3. and 4.

Transfer matrices: a natural tool

1. A.c. spectrum versus transfer matrices.

Spectral properties are related to generalized eigenfunctions [Carmona'83, Gilbert-Pearson '87, Last-Simon '99, Krutikov-Remling '01, Simon '07] and hence to transfer matrices.

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2. $G_{LB}(L, I)$ versus transfer matrices.

Recall: $G_{LB}(L, I) = \frac{1}{2\pi|I|} \int_I \mathcal{T}_L(E)\, \mathrm{d}E$ where $\mathcal{T}_L(E)$ is the transmission probability and can be expressed in terms of $(h_{\kappa,L} - E - i0)^{-1}$ via stationary scattering theory. We relate it to $(h_L - E - i0)^{-1}$ (and hence $T(L, E)$) via the resolvent formula [BJP '13]. One can actually show that

$$\mathcal{T}_L(E) \propto \| T(L, E)\|^{-2}.$$

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$$\mathcal{T}_L(E) \propto \|T(L,E)\|^{-2}.$$

3. $G_{Th}(L,I) \simeq |\mathrm{sp}(h_{\mathrm{per},L}) \cap I|$ versus transfer matrices.

$T(L,E) \in SL_2(\mathbb{R})$ and $E \in \mathrm{sp}(h_{\mathrm{per},L})$ iff $|\mathrm{Tr}\; T(L,E)| \leq 2$ (Floquet theory). We use it to get various estimates on $\|T(L,E)\|$, upper or lower bound, depending on whether E is in or out $\mathrm{sp}(h_{\mathrm{per},L})$.

The linear response regime

If $\mu_l = E$, $\mu_r = E + \varepsilon$, then $G_{lin}(L,E) := \lim_{\varepsilon \to 0} G_{LB}(L,I) = \frac{1}{2\pi} \mathcal{T}_L(E)$, i.e.

$$\omega_+(\mathcal{J}) \simeq \varepsilon \times G_{lin}(L,E) + o(1).$$

Let $\underline{\mathcal{I}} = \{E \mid \liminf G_{lin}(L,E) > 0\}$, $\bar{\mathcal{I}} = \{E \mid \limsup G_{lin}(L,E) > 0\}$.

Conjecture: $\underline{\mathcal{I}} = \mathrm{sp}_{\mathrm{ac,ess}}(-\Delta + v) = \bar{\mathcal{I}}$.

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The results of [BJP '13] combined with [GP '87, LS '99] show that

$$\underline{\mathcal{I}} \subset \mathrm{sp}_{\mathrm{ac,ess}}(-\Delta + v) \subset \bar{\mathcal{I}}.$$

The equality $\underline{\mathcal{I}} = \mathrm{sp}_{\mathrm{ac,ess}}(-\Delta + v)$ is equivalent to the Schrödinger conjecture, disproven in [Avila '15] in the framework of ergodic potentials.

The equality $\mathrm{sp}_{\mathrm{ac,ess}}(-\Delta + v) = \bar{\mathcal{I}}$ holds for ergodic potentials (follows from Kotani theory) and is an open question in general.

Plan

- Can be extended to Jacobi matrices
$$(hu)(n) = a_{n+1}u(n+1) + b_n u(n) + a_n u(n-1).$$
- More precise relation between the size of $\mathrm{sp}_{\mathrm{ac}}(-\Delta + v)$ and that of the periodic approximants: our proof shows
$$\limsup_{L\to\infty} |\mathrm{sp}(h_{\mathrm{per},L}) \cap I| \leq C|\mathrm{sp}_{\mathrm{ac}}(-\Delta + v) \cap I|^{\alpha}$$
where $C \simeq 16,5$ and $\alpha = 1/5$. On the full line [Gesztesy-Simon '96] or if v is ergodic [Last '94] one has $C = \alpha = 1$. Prove it on $\ell^2(\mathbb{Z}_+)$ for arbitrary v?
- Localized regime. Behavior of the conductances as $L \to \infty$. Relative scaling. Case of ergodic potentials and link with the Lyapunov exponents.
- Beyond the independent electron approximation: add local interactions inside the sample
$$\mathrm{d}\Gamma(h_{\kappa,L}) \rightsquigarrow \mathrm{d}\Gamma(h_{\kappa,L}) + \frac{\lambda}{2} \sum_{1\leq m,n\leq L} w(|m-n|)a^*(\delta_m)a^*(\delta_n)a(\delta_n)a(\delta_m).$$

THANK YOU !

The origin of Thouless conductance

Thouless conductance is originally “defined” (ET ’72) as $G_{Th} := \frac{\delta E}{\Delta E}$ where δE is a measure of sensitivity to B.C. and ΔE the level spacing of the system (at the Fermi energy where conduction takes place).

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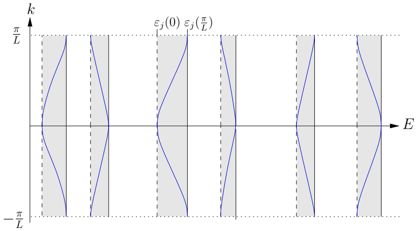
Various definitions have been proposed for δE, related to the variation of the energy levels $\varepsilon(k)$ of h_L with Bloch type B.C.

$$u(L+1) = \mathrm{e}^{ikL} u(1), \quad u(0) = \mathrm{e}^{-ikL} u(L).$$

One is the total variation of $\varepsilon(k)$ from periodic, $k = 0$, to antiperiodic, $k = \frac{\pi}{L}$, B.C.

The origin of Thouless conductance

The spectrum of $h_{\mathrm{per},L}$ consists in L bands, each corresponding to an eigenvalue $\varepsilon(k)$ of $h(k)$ as k varies from 0 to π/L.



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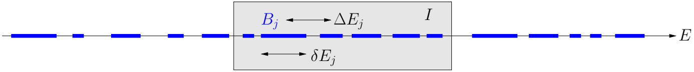

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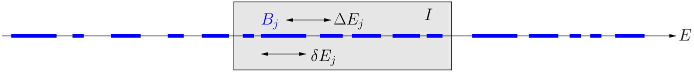

Given an energy window I, algebraic averages within I

$$\Delta E = \langle \Delta E_j \rangle = \frac{|I|}{\#\{j \mid B_j \subset I\}}, \qquad \delta E = \langle \delta E_j \rangle = \frac{|\mathrm{sp}(h_{\mathrm{per},L}) \cap I|}{\#\{j \mid B_j \subset I\}},$$

lead to $G_{Th}(L,I) \propto \dfrac{|\mathrm{sp}(h_{\mathrm{per},L}) \cap I|}{|I|}$. (First proposed by Last, PhD '94)