

# Conductances and a.c. spectrum

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

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# Plan

- 1 Introduction
- 2 Two notions of conductances
- 3 Conductances vs Spectrum
- 4 Concluding remarks

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

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

- 1 take  $h = -\Delta + v$  on  $\mathbb{Z}_+$ ,
- 2 restrict to  $\{1, \dots, L\}$ ,
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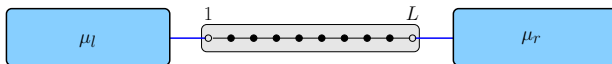
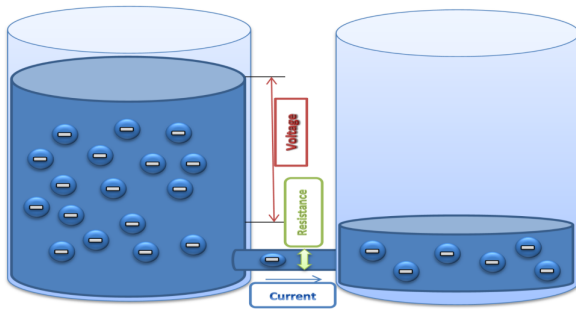
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**Physics literature:** transport theory of 1D systems goes back to 70's (Anderson, Thouless, Landauer,...)

**Math literature:** mostly absent until the last 10 years and the rigorous derivation of Landauer [AJPP '07, N '07] and Thouless [BJLP '15] formulas from first principles.

# An analogy



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## Setup: one electron data

A sample  $S$  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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**Sample:**  $\mathfrak{h}_L = \ell^2(\{1, \dots, L\})$  and  $h_L = -\Delta + v$ .

**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,

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

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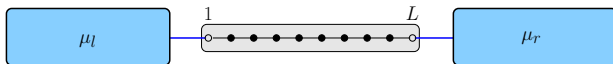
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**Coupled one electron system:**  $\mathfrak{h} = \mathfrak{h}_l \oplus \mathfrak{h}_L \oplus \mathfrak{h}_r$  and  $h_{\kappa,L} = h_{0,L} + \kappa h_T$  where

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



## Setup: many electrons

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

- Hilbert space: the fermionic Fock space  $\Gamma_-(\mathfrak{h}) = \bigoplus_{n=0}^{\infty} \wedge^n \mathfrak{h}$ .
- Hamiltonian: the second quantized operator  $H = d\Gamma(h_{\kappa,L})$ , 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  $\omega_0$  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  $N_r = d\Gamma(\mathbb{1}_r)$  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** [L '70], proven by [AJPP '07, N'07] provided  $\text{sp}_{\text{sc}}(h_{\kappa,L}) = \emptyset$ .

$$\omega_+(\mathcal{J}) := \lim_{T \rightarrow +\infty} \frac{1}{T} \int_0^T \omega_0(e^{itH} \mathcal{J} e^{-itH}) dt = \frac{1}{2\pi} \int_{\mu_l}^{\mu_r} \mathcal{T}_L(E) dE,$$

where  $\mathcal{T}_L(E)$  is the transmission probability at energy  $E$ .

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where  $\mathcal{T}_L(E)$  is the transmission probability at energy  $E$ .  
 Stationary scattering theory gives

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

**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  $h_{\kappa,L} = h_{\text{per},L}$  is the periodic extension of the sample, i.e. the  $L$ -periodic Schrödinger on  $\ell^2(\mathbb{Z})$  whose restriction to  $\{1, \dots, L\}$  is  $h_L$ .



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It amounts to take for the left, resp. right, reservoir the restriction of  $h_{\text{per},L}$  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  $E \in \text{sp}(h_{\text{per},L})$  and 0 otherwise. The Landauer-Büttiker formula thus gives

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

# The origin of Thouless conductance

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

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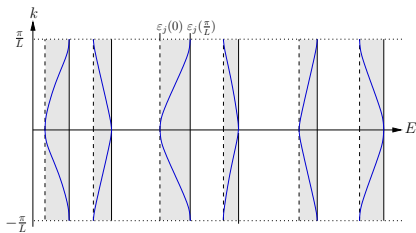
Various definitions have been proposed for  $\delta E$ , related to the variation of the energy levels  $\varepsilon(k)$  of  $h_L$  with Bloch type B.C.

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

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

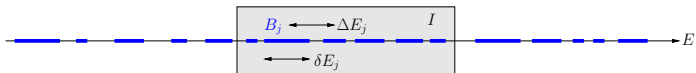
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The spectrum of  $h_{\text{per},L}$  consists in  $L$  bands, each corresponding to an eigenvalue  $\varepsilon(k)$  of  $h(k)$  as  $k$  varies from  $0$  to  $\pi/L$ .



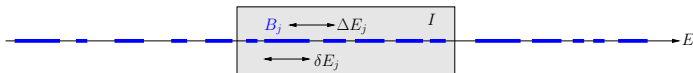
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Given an energy window  $I$ , algebraic averages within  $I$

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

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

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# 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



Physical characterization of conducting regime

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Physical characterization of conducting regime

Definition of transport:

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

# Main result

## Theorem (B.-Jakšić-Last-Pillet '15)

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

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

This gives a sharp characterization of ac spectrum:

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

Mathematical characterization of conducting regime



Physical characterization of conducting regime

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

## Main tool: transfer matrices

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

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

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### Theorem (B.-Jakšić-Last-Pillet '15)

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

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

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 the behavior of generalized eigenfunctions [C'83, GP '87, LS '99] and hence to transfer matrices.

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

Recall:  $G_{LB}(L, I) = \frac{1}{2\pi|I|} \int_I \mathcal{T}_L(E) dE$  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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## 3. $G_{Th}(L, I) \simeq |\text{sp}(h_{\text{per},L}) \cap I|$ versus transfer matrices.

$T(L, E) \in SL_2(\mathbb{R})$  and  $E \in \text{sp}(h_{\text{per},L})$  iff  $|\text{Tr } T(L, E)| \leq 2$  (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  $\text{sp}(h_{\text{per},L})$ .



# The linear response regime

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

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

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

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

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

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

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

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

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- Can be extended to Jacobi matrices

$$(hu)(n) = a_{n+1}u(n+1) + b_nu(n) + a_nu(n-1).$$

- More precise relation between the size of  $\text{sp}_{\text{ac}}(-\Delta + v)$  and that of the periodic approximants: our proof shows

$$\limsup_{L \rightarrow \infty} |\text{sp}(h_{\text{per},L}) \cap I| \leq C |\text{sp}_{\text{ac}}(-\Delta + v) \cap I|^\alpha$$

where  $C \simeq 16,5$  and  $\alpha = 1/5$ . On the full line [GS '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  $L \rightarrow \infty$ . Relative scaling. Case of ergodic potentials and link with the Lyapunov exponents.
- Beyond the independent electron approximation: add local interactions inside the sample

$$d\Gamma(h_{\kappa,L}) \rightsquigarrow d\Gamma(h_{\kappa,L}) + \frac{\lambda}{2} \sum_{1 \leq m, n \leq L} w(|m-n|) a^*(\delta_m) a^*(\delta_n) a(\delta_n) a(\delta_m).$$