Thouless conductance, Landauer-Büttiker currents and spectrum

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

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Plan

Thouless conductance

Introduced by Edwards and Thouless in 1972 as a criterion for localization in disordered (finite) systems (scaling theory of localization).

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Thouless conductance (or parameter) is “defined” as :

$$g_T := \frac{\delta E}{\Delta E}$$

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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Einstein relation gives $\sigma = e^2 D \dfrac{\mathrm{d}n}{\mathrm{d}E}$, with σ the conductivity and

$$\frac{\mathrm{d}n}{\mathrm{d}E} = \frac{1}{V \times \Delta E}$$

the density of states (per unit volume and unit energy).

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the density of states (per unit volume and unit energy).The conductance is thus ($A =$ cross-sectional arera, i.e. $V = A \times L$)

$$G = \frac{\sigma A}{L} \lesssim \frac{e^2}{\hbar} g_T,$$

with equality iff the uncertainty relation is an equality.
Even if it is heuristic, g_T is widely accepted as a measure of conductance.

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Consider a finite system described by a Jacobi matrix

$$(h(k)\psi)(x) = J_x \psi(x+1) + \lambda_x \psi(x) + J_{x-1}\psi(x-1)$$

from $x = 1$ to $x = L$ with Bloch type B.C.

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Various definitions have been proposed for δE,

- the variation of energy level from periodic to antiperiodic B.C., i.e. from $E(0)$ to $E(\frac{\pi}{L})$ where $E(k)$ is an eigenvalue of $h(k)$,
- the curvature $\displaystyle \frac{1}{L^2}\left|\frac{\mathrm{d}^2 E}{\mathrm{d}k^2}\right|_{k=0}$ of an eigenvalue at the edge of a band.

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We fix an interval I (e.g. small and around the Fermi energy) and consider algebraic averages within I

$$\Delta E = \frac{|I|}{\text{number of levels in } I}, \qquad \delta E = \frac{|{\rm sp}(h_{\rm per}) \cap I|}{\text{number of levels in } I}.$$

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This leads to the following

Definition

The Thouless conductance for the energy interval I is

$$g_T(I) = \frac{|\mathrm{sp}(h_{\mathrm{per}}) \cap I|}{|I|}.$$

g_T as a (dimensionless) conductance II

Let $I = (\mu_l, \mu_r)$ and assume the sample is connected to a left and right reservoir, at zero temperature and chemical potentials μ_l and μ_r.

$e_T(I) := |\mathrm{sp}(h_{\mathrm{per}}) \cap I|$, called Thouless energy, is identified with the current through the sample driven by the voltage difference between these reservoirs. Hence $g_T(I) = \dfrac{e_T(I)}{\mu_r - \mu_l}$ is the conductance.

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This identification holds provided some "optimal feeding" assumption holds: the time it takes for an electron to leave the right reservoir and occupy a vacant state is smaller than the time it takes to go through the sample. Otherwise the current should be less than $e_T(I)$.

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Our goal: make these statements precise, i.e. derive Thouless conductance formula from first principles of quantum statistical mechanics.

Quasi-free systems

Fermi gas in the independent electrons approximation:

- $\mathfrak{h}$ = one particle space.
- h = hamiltonian of one fermion.
- The total Hilbert space is then $\mathcal{H} = \Gamma_-(\mathfrak{h}) = \oplus_{n=0}^{\infty} \wedge^n \mathfrak{h}$.
- The hamiltonian is $H = \mathrm{d}\Gamma(h)$, i.e.

$$H\, f_1 \wedge \cdots \wedge f_n = \sum_{j=1}^{n} f_1 \wedge \cdots \wedge hf_j \wedge \cdots \wedge f_n.$$

- The algebra of observables $\mathcal{O} = \mathrm{CAR}(\mathfrak{h})$: the C^*-algebra generated by annihilation/creation operators $a(f)/a^*(f)$.

Electronic black box model

A sample $\mathcal{S}$ coupled to 2 reservoirs of electrons $\mathcal{R}_{l/r}$ described by a free fermi gas at thermal equilibrium (at inverse temperature β and chemical potential $\mu_{l/r}$) and in the independent electron approximation.

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One particle hamiltonian: $h = h_0 + h_T$ where

$$h_0 = h_l \oplus h_{\mathcal{S}} \oplus h_r, \quad h_T = |\chi_l\rangle\langle\psi_l| + |\psi_l\rangle\langle\chi_l| + |\chi_r\rangle\langle\psi_r| + |\psi_r\rangle\langle\chi_r|,$$

$(\mathfrak{h}_{\mathcal{S}}, h_{\mathcal{S}})$: finite-dimensional system (the sample), $\psi_{l/r} \in h_{\mathcal{S}}$.

$(\mathfrak{h}_{l/r}, h_{l/r})$: "free" reservoirs. Without loss of generality we may assume that $\delta_{l/r}$ are cyclic vectors for $h_{l/r}$. If $\nu_{l/r}$ is the spectral measure for $h_{l/r}$ and $\delta_{l/r}$ we may now take

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

Electronic black box model

The hamiltonian of the system is

$$H = \mathrm{d}\Gamma(h) = \mathrm{d}\Gamma(h_0) + a^*(\chi_l)a(\psi_l) + a^*(\psi_l)a(\chi_l) + a^*(\chi_r)a(\psi_r) + a^*(\psi_r)a(\chi_r),$$

and for any $A \in \mathcal{O}$, $\tau_t(A) := \mathrm{e}^{itH} A \mathrm{e}^{-itH}$, e.g. 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

$$\varrho = (1 + \mathrm{e}^{\beta(h_l - \mu_l)})^{-1} \oplus \rho_{\mathcal{S}} \oplus (1 + \mathrm{e}^{\beta(h_r - \mu_r)})^{-1},$$

i.e. ω_0 is such that

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

The current observable

The observable which describes the flux of particles out of $\mathcal{R}_r$ is

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

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 $h_r \simeq 0 \oplus 0 \oplus h_r$).

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We are interested in

$$\omega_+(\mathcal{J}_r) := \lim_{T\to+\infty} \frac{1}{T}\int_0^T \omega_0 \circ \tau_t(\mathcal{J}_r)\mathrm{d}t = \omega_+(\mathcal{J}_r),$$

where $\omega_+ = w* - \lim \dfrac{1}{T}\displaystyle\int_0^T \omega_0 \circ \tau^t$ is the NESS of the system (if it exists).

Landauer-Büttiker formula

The wave operators $w_\pm := s - \lim_{t\to\pm\infty} \mathrm{e}^{ith}\mathrm{e}^{-ith_0}\mathbb{1}_{\mathrm{ac}}(h_0)$ exist and are complete. The scattering matrix $s = w_+^* w_-$ acts as multiplication by

$$s(E) = \begin{pmatrix} s_{ll}(E) & s_{lr}(E) \\ s_{rl}(E) & s_{rr}(E) \end{pmatrix}.$$

$\mathcal{T}(E) := |s_{lr}(E)|^2 = |s_{rl}(E)|^2$ is the transmission probability between the reservoirs at energy E.

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Theorem (AJPP '07)

If $\mathrm{sp}_{\mathrm{sc}}(h) = \emptyset$, $\omega_+(A) := \lim \frac{1}{T}\int_0^T \omega_0 \circ \tau^t(A)\mathrm{d}t$ *exists* $\forall A \in \mathcal{O}$ *and*

$$\omega_+(\mathcal{J}_r) = \frac{1}{2\pi}\int_{\mathbb{R}} \mathcal{T}(E) \times \left(\frac{1}{1+\mathrm{e}^{\beta(E-\mu_r)}} - \frac{1}{1+\mathrm{e}^{\beta(E-\mu_l)}}\right)\mathrm{d}E.$$

Remark : $\mathcal{T}(E) = 4|\langle\psi_l, (h-E-\mathrm{i}0)^{-1}\psi_r\rangle|^2\,\mathrm{Im}F_l(E)\,\mathrm{Im}F_r(E)$
where $F_{l/r}(E) := \langle\chi_{l/r}, (h_{l/r}-E-\mathrm{i}0)^{-1}\chi_{l/r}\rangle$. Hence $\mathcal{T}(E) = 0$ if $E \notin \mathrm{sp}_{\mathrm{ac}}(h_\ell) \cap \mathrm{sp}_{\mathrm{ac}}(h_r)$.

Landauer conductance

Assume we are at zero temperature and $\mu_l < \mu_r$, the Landauer conductance is then

$$g_L(l) = \frac{\omega_+(\mathcal{J}_r)}{\mu_r - \mu_l} = \frac{1}{2\pi(\mu_r - \mu_l)} \int_{\mu_l}^{\mu_r} \mathcal{T}(E)\,\mathrm{d}E.$$

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Take now as a sample our finite system, i.e. $\mathfrak{h}_\mathcal{S} = \ell^2([1, L])$, and

$$(h_\mathcal{S}\psi)(x) = J_x\psi(x+1) + \lambda_x\psi(x) + J_{x-1}\psi(x-1)$$

with Dirichlet boundary condition and $\psi_l = \delta_1$, $\psi_r = \delta_L$.

Crystal EBB

Assume that the left/right reservoir are such that $h = h_{\rm per}$, i.e. the left, resp. right, reservoir is the restriction of $h_{\rm per}$ to $\ell^2((-\infty, 0])$, resp. $\ell^2([L+1, \infty))$, with Dirichlet B.C. and $\chi_{l/r} = J_{0/L}\delta_{0/L+1}$, so-called "matching wire" (Economou-Soukoulis '91) or "optimal feeding".

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One then have $\mathcal{T}(E) = 1$ for $E \in {\rm sp}(h_{\rm per})$ while $\mathcal{T}(E) = 0$ for $E \notin {\rm sp}(h_{\rm per})$ so that

$$g_L(I) = \frac{1}{2\pi(\mu_r - \mu_l)} \int_{\mu_l}^{\mu_r} \mathcal{T}(E)\,{\rm d}E = \frac{1}{2\pi} \frac{|{\rm sp}(h_{\rm per}) \cap I|}{|I|} = \frac{1}{2\pi} g_T(I),$$

where $I = (\mu_l, \mu_r)$.

Remark: if optimal feeding fails then the current should be less, i.e. $g_T(I)$ should give an upper bound.

Crystallined Landauer-Büttiker formula

We come back to arbitrary reservoirs but now consider the following sample. Given an integer N:

$h_{\mathcal{S}}^{(N)}$ is the restriction of $h_{\rm per}$ to $\ell^2([1, NL])$, i.e. a finite Jacobi matrix whose coefficients are L-periodic, with Dirichlet B.C. and with $\psi_l = \delta_1$ and $\psi_r = \delta_{NL}$.

We denote by $\omega_+^{(N)}(\mathcal{J}_r^{(N)})$ the corresponding current expectation value in the NESS. We are interested in its large N limit.

Remark: Similar idea of "crystallizing" or "periodizing" appears in a band random matrix approach by Cassati-Guarneri-Maspero ('97).

Crystallined Landauer-Büttiker formula

Let $h_{\rm per}^{(l)}$, resp. $h_{\rm per}^{(r)}$, denote the restriction of $h_{\rm per}$ to $\ell^2((-\infty,0])$, resp. $\ell^2([1,\infty))$, with Dirichlet B.C. We denote by $m_{l/r}$ its Weyl m-function:

$$m_l(E) := \langle \delta_0, (h_{\rm per}^{(l)} - E - \mathrm{i}0)^{-1}\delta_0\rangle, \quad m_r(E) := \langle \delta_1, (h_{\rm per}^{(r)} - E - \mathrm{i}0)^{-1}\delta_1\rangle.$$

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The crystalline transmission coefficient is defined, for $E \in {\rm sp}(h_{\rm per})$, as

$$\mathcal{T}_{\rm crys}(E) = \frac{4J_0^2|1-J_0^2 m_l(E)m_r(E)|^2\,{\rm Im}F_l(E)\,{\rm Im}F_r(E)}{J_0^4|1-m_r(E)F_l(E)|^2|1-m_l(E)F_r(E)|^2 - |J_0^2 m_l(E)-F_l(E)|^2|J_0^2 m_r(E)-F_r(E)|^2}.$$

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Property: $0 \le \mathcal{T}_{\rm crys}(E) \le 1$.

For a crystal EBB $F_{l/r}(E) = J_0^2 m_{l/r}(E)$ and $\mathcal{T}_{\rm crys}(E) \equiv 1$.

Crystallined Landauer-Büttiker formula

Theorem

$$\begin{aligned}\langle \mathcal{J}_r \rangle_{\mathrm{crys}} &:= \lim_{N\to\infty} \omega_+^{(N)}(\mathcal{J}_r^{(N)}) \\ &= \frac{1}{2\pi}\int_{\mathbb{R}} \mathcal{T}_{\mathrm{crys}}(E) \times \left(\frac{1}{1+\mathrm{e}^{\beta(E-\mu_r)}} - \frac{1}{1+\mathrm{e}^{\beta(E-\mu_l)}} \right) \mathrm{d}E.\end{aligned}$$

In particular, at zero temperature,

$$\langle \mathcal{J}_r \rangle_{\mathrm{crys}} = \frac{1}{2\pi}\int_{\mu_l}^{\mu_r} \mathcal{T}_{\mathrm{crys}}(E)\mathrm{d}E \;\leq\; \frac{1}{2\pi} e_T((\mu_l,\mu_r)).$$

Thouless energy gives an upper bound for Landauer current, with equality iff $\mathcal{T}_{\mathrm{crys}}(E) \equiv 1$ on (μ_l, μ_r). Optimal feeding is identified to reflectionless transport between the reservoirs. It holds for example for crystal EBB (matching wires).

Thouless conductance vs ac spectrum

Thouless's idea is that a system exhibits localization if $g_T(I)$ decays to 0 with L.

Let h_∞ be a Jacobi matrix on $\ell^2(\mathbb{Z}_+)$ and $h_{\rm per}^L$ its periodic approximant of size L, i.e. $h_{\rm per}^L$ coincide with h_∞ on $[1, L]$ and then is extended periodically.

How does $g_T^L(I) := \dfrac{|{\rm sp}(h_{\rm per}^L) \cap I|}{|I|}$ behaves as $L \to \infty$?

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Theorem

If I is an open interval such that $\mathrm{sp}_{\mathrm{ac}}(h_\infty) \cap I = \emptyset$ then $g_T^L(I) \to 0$.
If moreover h_∞ is ergodic then it is an equivalence.

First part follows from Gesztesy-Simon ('96) results, the second part was proven by Last in is thesis ('94).

Landauer conductance vs ac spectrum

In the Landauer approach, instead of first crystallizing and then taking the size of the sample to infinity, one may simply take the size of the sample to infinity.

That is, consider the EBB model where the sample is the restriction of h_∞ to $[1, L]$ and let $\omega_{+,L}(\mathcal{J}_{r,L})$ denote the corresponding expectation value of the charge current in the steady state.

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Theorem

If I is an open interval such that $\liminf_{L\to\infty} \omega_{+,L}(\mathcal{J}_{r,L}) = 0$ then $\mathrm{sp}_{\mathrm{ac}}(h_\infty) \cap I = \emptyset$.

Remark: The reservoirs have to contain I in their ac spectra but otherwise arbitrary.
The proof uses the connection between $\omega_{+,L}(\mathcal{J}_{r,L})$ and the transfer matrices of h_∞ combined with results by Last-Simon ('99).