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Landauer-Büttiker and Thouless conductance

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Dedicated to the memory of Markus Büttiker

Abstract. In the independent electron approximation, the average (energy/charge/entropy) current flowing through a finite sample $\mathcal{S}$ connected to two electronic reservoirs can be computed by scattering theoretic arguments which lead to the famous Landauer-Büttiker formula. Another well known formula has been proposed by Thouless on the basis of a scaling argument. The Thouless formula relates the conductance of the sample to the width of the spectral bands of the infinite crystal obtained by periodic juxtaposition of $\mathcal{S}$. In this spirit, we define Landauer-Büttiker crystalline currents by extending the Landauer-Büttiker formula to a setup where the sample $\mathcal{S}$ is replaced by a periodic structure whose unit cell is $\mathcal{S}$. We argue that these crystalline currents are closely related to the Thouless currents. For example, the crystalline heat current is bounded above by the Thouless heat current, and this bound saturates iff the coupling between the reservoirs and the sample is reflectionless. Our analysis leads to a rigorous derivation of the Thouless formula from the first principles of quantum statistical mechanics.

1 Introduction

Recent rigorous formulations of the Landauer-Büttiker formula [AJPP, BSP, CJM, N] in the framework of nonequilibrium quantum statistical mechanics have opened the way to the mathematical study of a variety of related transport phenomena in quantum mechanics [GJW, JLPa, JLPi]. This paper is a continuation of this line of research. Our main goal here is to provide a mathematically rigorous proof of the celebrated Thouless conductance formula.

This paper is organized as follows. In Section 1.1 we review the Electronic Black Box Model and the corresponding Landauer-Büttiker formula. These topics have been discussed from both technical and pedagogical point of view in [AJPP, BSP] and the reader may consult these works for additional information. The notions of Thouless energy and Thouless conductance are reviewed in Section 1.2. Our main results are stated in Section 2. The proofs are given in Section 3.

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1.1 The Electronic Black Box Model and the Landauer-Büttiker formula

The Electronic Black Box Model (abbreviated EBBM) describes a finite sample $\mathcal{S}$ connected to two infinitely extended electronic reservoirs $\mathcal{R}_{l/r}$ (where l/r stands for left/right) in the independent electron approximation. The coupling between the sample and the reservoirs allows for a flow of energy/charge/entropy through the joint system $\mathcal{R}_l + \mathcal{S} + \mathcal{R}_r$.

We shall restrict our attention to one-dimensional samples in the tight binding approximation. Thus, the sample $\mathcal{S}$ is a free Fermi gas with one-particle Hilbert space $\mathfrak{h}_{\mathcal{S}} = \ell^2(Z_L)$, where $Z_L = [1, L] \cap \mathbb{Z}$ is a finite lattice. Its Hamiltonian $h_{\mathcal{S}}$ is a Jacobi matrix with parameters $\{J_x\}_{1\leq x<L}$, $\{\lambda_x\}_{1\leq x\leq L}$,

$$(h_{\mathcal{S}}u)(x) = J_x u(x+1) + J_{x-1}u(x-1) + \lambda_x u(x), \qquad x \in Z_L, \tag{1.1}$$

and Dirichlet boundary condition $u(0) = u(L+1) = 0$. The reservoir $\mathcal{R}_{l/r}$ is a free Fermi gas with one-particle Hilbert space $\mathfrak{h}_{l/r}$ and one-particle Hamiltonian $h_{l/r}$. The one-particle Hilbert space and Hamiltonian of the composite system $\mathcal{R}_l + \mathcal{S} + \mathcal{R}_r$ are

$$\mathfrak{h} = \mathfrak{h}_l \oplus \mathfrak{h}_{\mathcal{S}} \oplus \mathfrak{h}_r,$$

$$h_0 = h_l \oplus h_{\mathcal{S}} \oplus h_r.$$

The coupling of the sample with the reservoir $\mathcal{R}_{l/r}$ is realized by the hopping Hamiltonian

$$v_{l/r} = |\chi_{l/r}\rangle\langle\psi_{l/r}| + |\psi_{l/r}\rangle\langle\chi_{l/r}|,$$

where $\chi_{l/r} \in \mathfrak{h}_{l/r}$ is a unit vector while $\psi_l = \delta_1$ and $\psi_r = \delta_L$ are Kronecker delta functions in $\mathfrak{h}_{\mathcal{S}}$. The one-particle Hamiltonian of the coupled system is

$$h = h_0 + \kappa v = h_0 + \kappa(v_l + v_r),$$

where $\kappa \neq 0$ is the coupling strength. As observed in [BJP], for the purposes of discussing transport properties of the coupled system $\mathcal{R}_l + \mathcal{S} + \mathcal{R}_r$ one may assume, without loss of generality, that $\chi_{l/r}$ is a cyclic vector for $h_{l/r}$. Hence, passing to the spectral representation we may assume that $h_{l/r}$ acts as multiplication by E on

$$\mathfrak{h}_{l/r} = L^2(\mathbb{R}, \mathrm{d}\nu_{l/r}(E)),$$

where $\nu_{l/r}$ is the spectral measure of $h_{l/r}$ associated to $\chi_{l/r}$. Moreover, in this representation one has $\chi_{l/r}(E) = 1$ and $\nu_{l/r}(\mathbb{R}) = 1$.

Let $\Gamma_-(\mathfrak{h})$ be the fermionic Fock space over $\mathfrak{h}$ and denote by $a(f)/a^*(f)$ the annihilation/creation operator on $\Gamma_-(\mathfrak{h})$ associated to $f \in \mathfrak{h}$. The algebra of observables of the EBBM is the C^*-algebra $\mathcal{O}$ of all bounded operators on $\Gamma_-(\mathfrak{h})$ generated by the identity I and $\{a^*(f)a(g) \mid f, g \in \mathfrak{h}\}$.

Let $H = \mathrm{d}\Gamma(h)$ be the second quantized Hamiltonian. The map

$$\tau^t(a^*(f)a(g)) = \mathrm{e}^{\mathrm{i}tH}a^*(f)a(g)\mathrm{e}^{-\mathrm{i}tH} = a^*(\mathrm{e}^{\mathrm{i}th}f)a(\mathrm{e}^{\mathrm{i}th}g),$$

extends to a strongly continuous group of $*$-automorphisms of $\mathcal{O}$ and the pair $(\mathcal{O}, \tau^t)$ is a C^*-dynamical system. The states of the EBBM are normalized positive linear functionals on $\mathcal{O}$.

Since we are dealing with independent electrons, quasi-free states on $\mathcal{O}$ will be of particular relevance. Let ρ be a self-adjoint operator of $\mathfrak{h}$ such that $0 \leq \rho \leq I$. The gauge-invariant quasi-free state of density ρ is the unique state ω_ρ on $\mathcal{O}$ satisfying

$$\omega_\rho(a^*(f_1)\cdots a^*(f_n)a(g_m)\cdots a(g_1)) = \delta_{n,m}\det\{\langle g_i, \rho f_j\rangle\},$$

for any integers n, m and all $f_1, \ldots, f_n, g_1, \ldots, g_m \in \mathfrak{h}$.

The initial state ω_0 of the EBBM is the gauge-invariant quasi-free state of density

$$\rho_0 = \rho_l \oplus \rho_{\mathcal{S}} \oplus \rho_r,$$

where $\rho_{l/r}$ is the operator of multiplication by the Fermi-Dirac density

$$\rho_{l/r}(E) = \frac{1}{1 + \mathrm{e}^{\beta_{l/r}(E-\mu_{l/r})}}.$$

In other words, the reservoir $\mathcal{R}_{l/r}$ is initially in thermal equilibrium at inverse temperature $\beta_{l/r} > 0$ and chemical potential $\mu_{l/r} \in \mathbb{R}$. None of our results depends on the particular choice of the initial density $\rho_{\mathcal{S}}$ of the sample.

The EBBM is the quantum dynamical system $(\mathcal{O}, \tau^t, \omega_0)$.

The basic questions regarding this system concern its behavior in the large time limit $t \to \infty$. To deal with this limit we observe that the initial state $\omega_0 = \omega_{\rho_0}$ evolves in time as

$$\omega_t = \omega_0 \circ \tau^t = \omega_{\rho_t},$$

where the density at time t is given by

$$\rho_t = \mathrm{e}^{-\mathrm{i}th}\rho_0\mathrm{e}^{\mathrm{i}th}.$$

One expects that $\omega_t \to \omega_+$ as $t \to \infty$, where the non-equilibrium steady state ω_+ carries energy/charge/entropy current induced by the initial temperature/chemical potential differential. These currents can be expressed by Landauer-Büttiker formulas involving transmission properties of individual electrons evolving under the dynamics generated by the one-particle Hamiltonian h. These heuristics is mathematically formalized as follows.

The observables describing energy and charge current out of $\mathcal{R}_{l/r}$ are

$$\Phi_{l/r} = \mathrm{d}\Gamma(-\mathrm{i}[h, h_{l/r}]) = \kappa\left(a^*(\mathrm{i}h_{l/r}\chi_{l/r})a(\psi_{l/r}) + a^*(\psi_{l/r})a(\mathrm{i}h_{l/r}\chi_{l/r})\right),$$

$$\mathcal{I}_{l/r} = \mathrm{d}\Gamma(-\mathrm{i}[h, 1_{l/r}]) = \kappa\left(a^*(\mathrm{i}\chi_{l/r})a(\psi_{l/r}) + a^*(\psi_{l/r})a(\mathrm{i}\chi_{l/r})\right).$$

The entropy current associated to the heat flux dissipated into the reservoirs is

$$\mathcal{J} = -\beta_l(\Phi_l - \mu_l\mathcal{I}_l) - \beta_r(\Phi_r - \mu_r\mathcal{I}_r).$$

The transmittance of the sample is the function [1]

$$\mathbb{R} \ni E \mapsto \mathcal{T}(E) = 4\kappa^4 |\langle \psi_l, (h - E - \mathrm{i}0)^{-1} \psi_r \rangle|^2 \operatorname{Im} F_l(E) \operatorname{Im} F_r(E), \tag{1.2}$$

where

$$F_{l/r}(E) = \langle \chi_{l/r}, (h_{l/r} - E - \mathrm{i}0)^{-1} \chi_{l/r} \rangle. \tag{1.3}$$

Note that $\operatorname{Im} F_{l/r}(E) \geq 0$ and [2]

$$\{E \in \mathbb{R} \,|\, \mathcal{T}(E) > 0\} = \Sigma_l \cap \Sigma_r, \tag{1.4}$$

where

$$\Sigma_{l/r} = \{E \in \mathbb{R} \,|\, \operatorname{Im} F_{l/r}(E) > 0\} \tag{1.5}$$

is the essential support of the absolutely continuous spectrum of $h_{l/r}$.

For $E \in \mathbb{R}$ we set

$$\zeta_{l/r}(E) = \beta_{l/r}(E - \mu_{l/r}), \qquad \Delta_{l/r}(E) = \rho_{l/r}(E) - \rho_{r/l}(E),$$

and

$$\varsigma(E) = (\zeta_r(E) - \zeta_l(E))\Delta_l(E) = (\zeta_l(E) - \zeta_r(E))\Delta_r(E).$$

Note that if $\beta_l = \beta_r$ and $\mu_l = \mu_r$ then $\varsigma(E)$ vanishes identically but that it is strictly positive for all $E \in \mathbb{R}$ otherwise.

Our basic assumption in the following is:

> **Assumption A.** The one-particle Hamiltonian h has no singular continuous spectrum.

The starting point of this paper is the following result [AJPP].

Theorem 1.1 *Suppose that Assumption* **A** *holds. Then for all $A \in \mathcal{O}$ the limit*

$$\omega_+(A) = \lim_{t \to \infty} \frac{1}{t} \int_0^t \omega_s(A) \mathrm{d}s,$$

exists and defines a state ω_+ on $\mathcal{O}$. Moreover, the following formulas for the average steady currents hold:

$$\begin{aligned} \langle \Phi_{l/r} \rangle_+ &= \omega_+(\Phi_{l/r}) = \frac{1}{2\pi} \int_{\mathbb{R}} \mathcal{T}(E) E \Delta_{l/r}(E) \mathrm{d}E, \\ \langle \mathcal{I}_{l/r} \rangle_+ &= \omega_+(\mathcal{I}_{l/r}) = \frac{1}{2\pi} \int_{\mathbb{R}} \mathcal{T}(E) \Delta_{l/r}(E) \mathrm{d}E, \\ \langle \mathcal{J} \rangle_+ &= \omega_+(\mathcal{J}) = \frac{1}{2\pi} \int_{\mathbb{R}} \mathcal{T}(E) \varsigma(E) \mathrm{d}E. \end{aligned} \tag{1.6}$$

[1] This function is defined for Lebesgue a.e. $E \in \mathbb{R}$.

[2] This identity is understood modulo sets of Lebesgue measure zero.

We finish this section with a number of remarks regarding this result.

Remark 1. Theorem 1.1 deals with the simplest non-trivial setting in the study of electronic transport in the independent electron approximation. Various generalizations of this setting and of Theorem 1.1 can be found in [AJPP, N, BSP].

Remark 2. We have chosen units in such a way that the electronic charge e, the reduced Planck constant $\hbar$, and the Boltzmann constant k_B are unity. The energy, charge, and entropy currents in the above formulas are expressed in units of $1/\hbar$, $e/\hbar$ and $k_B/\hbar$. Note also that these formulas do not include the spin degeneracy which should be accounted for by a factor 2.

Remark 3. If Assumption **A** is replaced by the stronger assumption that h has no singular spectrum, then

$$\omega_+(A) = \lim_{t\to\infty} \omega_t(A),$$

holds for all $A \in \mathcal{O}$.

Remark 4. If $\beta_l = \beta_r = \beta$ and $\mu_l = \mu_r = \mu$, then ω_+ is the thermal equilibrium state of the coupled system $\mathcal{R}_l + \mathcal{S} + \mathcal{R}_r$ for the given intensive thermodynamic parameters, i.e., the quasi-free state of density

$$\rho_{\beta,\mu} = \frac{1}{1 + \mathrm{e}^{\beta(h-\mu)}}.$$

In this case, all currents vanish in average. In the following we shall exclude this possibility and assume that $\beta_l \neq \beta_r$ or/and $\mu_l \neq \mu_r$. The state ω_+ is then a non-equilibrium steady state of the EBBM and (1.6) are the Landauer-Büttiker formulas for the steady state currents.

Remark 5. Apart from the choice of the intensive thermodynamic parameters $\beta_{l/r}$ and $\mu_{l/r}$, the transmission coefficient $\mathcal{T}(E)$ completely determines the steady state currents. It follows from (1.4) that the steady state currents are non-vanishing iff the Lebesgue measure $|\Sigma_l \cap \Sigma_r|$ of the set $\Sigma_l \cap \Sigma_r$ is strictly positive, i.e., iff there exists an open scattering channel between the left and the right reservoir. Note the obvious conservation laws

$$\omega_+(\Phi_l) + \omega_+(\Phi_r) = 0, \qquad \omega_+(\mathcal{I}_l) + \omega_+(\mathcal{I}_r) = 0.$$

Entropy balance in the steady state ω_+ implies that

$$\langle \mathcal{J} \rangle_+ = -\beta_l(\langle \Phi_l \rangle_+ - \mu_l \langle \mathcal{I}_l \rangle_+) - \beta_r(\langle \Phi_r \rangle_+ - \mu_r \langle \mathcal{I}_r \rangle_+),$$

coincides with the rate of entropy production in $\mathcal{S}$ [AJPP]. It follows from the above observation that $\langle \mathcal{J} \rangle_+ \geq 0$, and that the inequality is strict iff $|\Sigma_l \cap \Sigma_r| > 0$.

Remark 6. The proof of Theorem 1.1 is based on the scattering theory of the pair (h, h_0) and elucidates the physical meaning of $\mathcal{T}(E)$. It follows from the trace class scattering theory that the wave operators [3]

$$w_\pm = \mathrm{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}th} \mathrm{e}^{-\mathrm{i}th_0} 1_{\mathrm{ac}}(h_0),$$

[3] $1_{\mathrm{ac}}(h_0)$ is the spectral projection on the absolutely continuous part of the spectrum of h_0.

exist and are complete. The scattering matrix $s = w_+^* w_-$ is a unitary operator on

$$\mathfrak{h}_{\mathrm{ac}}(h_0) = \operatorname{Ran} 1_{\mathrm{ac}}(h_0) = \operatorname{Ran} 1_{\mathrm{ac}}(h_l) \oplus \operatorname{Ran} 1_{\mathrm{ac}}(h_r),$$

and acts as the operator of multiplication by a unitary 2×2 matrix

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

One then has

$$\mathcal{T}(E) = |s_{lr}(E)|^2 = |s_{rl}(E)|^2,$$

i.e., the transmittance $\mathcal{T}(E)$ is the transmission probability between the left and right reservoir at energy E.

Remark 7. An additional insight into $\mathcal{T}(E)$ can be obtained by taking into account the spatial structure of the reservoirs. Suppose that the reservoirs are non-trivial in the sense that the measures $\nu_{l/r}$ have non-vanishing absolutely continuous component. The standard orthogonal polynomial construction (see Theorem I.2.4 in [Si]) provides a unitary operator $U : \mathfrak{h} \to \ell^2(\mathbb{Z})$ such that the following holds:

(i) $U\mathfrak{h}_l = \ell^2(]-\infty, 0] \cap \mathbb{Z})$, $U\mathfrak{h}_{\mathcal{S}} = \mathfrak{h}_{\mathcal{S}}$ and $U\mathfrak{h}_r = \ell^2([L+1, \infty[\cap\mathbb{Z})$.

(ii) There is a Jacobi matrix on $\ell^2(]-\infty, 0] \cap \mathbb{Z})$, with parameters $\{J_x\}_{x<0}$, $\{\lambda_x\}_{x\leq 0}$ and Dirichlet boundary condition such that for $u \in \ell^2(]-\infty, 0] \cap \mathbb{Z})$

$$(Uh_l U^* u)(x) = J_x u(x+1) + J_{x-1} u(x-1) + \lambda_x u(x), \qquad (x \leq 0, u(1) = 0).$$

(iii) $Uh_{\mathcal{S}} U^* = h_{\mathcal{S}}$.

(iv) There is a Jacobi matrix on $\ell^2([L+1, \infty[\cap\mathbb{Z})$, with parameters $\{J_x\}_{x>L}$, $\{\lambda_x\}_{x>L}$ and Dirichlet boundary condition such that for $u \in \ell^2([L+1, \infty[\cap\mathbb{Z})$

$$(Uh_r U^* u)(x) = J_x u(x+1) + J_{x-1} u(x-1) + \lambda_x u(x), \qquad (x > L, u(L) = 0).$$

(v) $U\chi_l = \delta_0$ and $U\chi_r = \delta_{L+1}$.

(vi) If $J_0 = J_L = \kappa$, then for $u \in \ell^2(\mathbb{Z})$

$$(UhU^* u)(x) = J_x u(x+1) + J_{x-1} u(x-1) + \lambda_x u(x).$$

It follows that our EBBM is unitarily equivalent to a Jacobi matrix EBBM on $\ell^2(\mathbb{Z})$.

For $z \in \mathbb{C}_+$ let $u_{l/r}(\,\cdot\,, z)$ be the unique solution of the equation

$$J_x u_{l/r}(x+1, z) + J_{x-1} u_{l/r}(x-1, z) + \lambda_x u_{l/r}(x, z) = z u_{l/r}(x, z), \tag{1.7}$$

that is square summable at $\pm\infty$ and normalized by $u_{l/r}(0,z)=1$. For all $x\in\mathbb{Z}$ and Lebesgue a.e. $E\in\mathbb{R}$ the limit

$$\lim_{\epsilon\downarrow 0} u_{l/r}(x,E+\mathrm{i}\epsilon)=u_{l/r}(x,E),$$

exists, is finite, and solves (1.7) with $z=E$. For Lebesgue a.e. $E\in\Sigma_r$ the solution $u_r(E)$ is not a multiple of a real solution and so $\overline{u_r(E)}$ is also a solution of (1.7) linearly independent of $u_r(E)$. Hence, for Lebesgue a.e. $E\in\Sigma_r$ one has

$$u_l(E)=\alpha(E)\overline{u_r(E)}+\beta(E)u_r(E).$$

The spectral reflection probability of [GNP, GS] is

$$R_r(E)=\left|\frac{\beta(E)}{\alpha(E)}\right|^2.$$

One extends R_r to $\mathbb{R}$ by setting $R_r(E)=1$ for $E\notin\Sigma_r$. $R_l(E)$ is defined analogously. A simple computation (see Section 5 in [JLPa]) gives

$$R_r(E)=R_l(E)=|s_{ll}(E)|^2=|s_{rr}(E)|^2.$$

Hence,

$$\mathcal{T}(E)=1-R_r(E)=1-R_l(E),$$

is the spectral transmission probability at the energy E.

1.2 The Thouless energy and the Thouless conductance formula

We start with a review of the notions of Thouless energy and conductance as discussed in the physics literature. We follow [La] and our main goal is to extract mathematically well-defined quantities that correspond to these heuristic notions.

1.2.1 Heuristics

Let δt be the typical time spent in $\mathcal{S}$ by an electron on its journey from one reservoir to the other. The Mandelstam-Tamm time-energy uncertainty relation $\delta E\,\delta t\gtrsim 1$ ([MT], see also [FP, Bu]) imposes a lower bound on the energy spread δE of the electron wave function. This sets the *Thouless energy* scale $E_{\mathrm{Th}}\sim\delta E$ [Th]. Assuming a diffusive behavior, one has $L^2\sim D\delta t$ where L is the sample size and D the diffusion constant, and hence

$$E_{\mathrm{Th}}\gtrsim\frac{D}{L^2}.$$

Einstein's relation

$$\sigma=D\varrho\lesssim L^2E_{\mathrm{Th}}\varrho,$$

further links D to the conductivity σ of the sample and its density of states ϱ. Finally, ϱ relates to the typical energy level spacing ΔE of the sample as

$$\varrho L \Delta E \sim 1.$$

It follows that

$$\sigma \lesssim L \frac{E_{\mathrm{Th}}}{\Delta E},$$

and hence that the conductance $g = L^{-1}\sigma$ of the one-dimensional sample satisfies

$$g \lesssim g_{\mathrm{Th}} = \frac{E_{\mathrm{Th}}}{\Delta E}. \tag{1.8}$$

The quantity at the r.h.s. of this formula is known as the *Thouless conductance*. Although the above derivation is extremely heuristic in nature, the Thouless conductance g_{Th} and the closely related Thouless energy E_{Th} are widely accepted by both theoretical and experimental physicists and play an important role in the scaling theory of localization [AALR].

The above argument and the resulting inequality on the l.h.s. of (1.8) suggest that we should consider g_{Th} as an upper bound on the conductance of the sample $\mathcal{S}$. Indeed, for such a microscopic system the conductance is not an intrinsic property of the sample, but depends also on the reservoirs and the nature of the coupling, which determines the reservoir's ability to feed the available energy levels of the sample. Thus, one expects that saturation of the Thouless bound (1.8) occurs for optimal feeding of the sample by the reservoirs, a property of the joint system $\mathcal{R}_l + \mathcal{S} + \mathcal{R}_r$ which we shall try to elucidate in the remaining part of this paper (see Remarks 1 and 4 after Theorem 2.3).

1.2.2 The crystal model

There is a simple way to make the sample transparent to incoming electrons and hence to ensure its optimal feeding: it suffices to implement the reservoirs in such a way that the joint system $\mathcal{R}_l + \mathcal{S} + \mathcal{R}_r$ is periodic. We shall call *crystalline EBBM* the model obtained by repeating the sample so as to obtain a periodic crystal with unit cell $\mathcal{S}$ (a construction closely related to the scaling argument of [ET]).

Consider the periodic Jacobi matrix h_{crystal} on $\ell^2(\mathbb{Z})$ obtained by extending the Jacobi parameters $\{\lambda_x\}_{1\le x\le L}$ and $\{J_x\}_{1\le x<L}$ of the sample Hamiltonian $h_{\mathcal{S}}$ to the entire lattice $\mathbb{Z}$ by setting $J_L = \kappa_{\mathcal{S}}$ and

$$J_{x+nL} = J_x, \qquad \lambda_{x+nL} = \lambda_x,$$

for any $n \in \mathbb{Z}$ and $x \in Z_L$. The internal coupling constant $\kappa_{\mathcal{S}}$ is a priori an arbitrary parameter, except for the obvious constraint $\kappa_{\mathcal{S}} \neq 0$. In practice it will be determined by the physics of the problem. In a model where the sample parameters J_x are independent copies of a random

variable, $\kappa_{\mathcal{S}}$ will be another instance of this variable. If $h_{\mathcal{S}}$ is a discrete Schrödinger operator with $J_x = J$ for all $x \in Z_L$ the choice of $\kappa_{\mathcal{S}} = J$ appears natural.

In the crystaline EBBM model, the single particle Hilbert spaces of the reservoirs are $\mathfrak{h}_l = \ell^2(]-\infty, 0] \cap \mathbb{Z})$ and $\mathfrak{h}_r = \ell^2([L+1, \infty[\cap\mathbb{Z})$, the corresponding single particle Hamiltonians are Jacobi matrices with parameters $\{\{J_x\}_{x<0}, \{\lambda_x\}_{x<0}\}$, $\{\{J_x\}_{x>L}, \{\lambda_x\}_{x>L}\}$ and Dirichlet boundary condition, $\chi_l = \delta_0$, $\chi_r = \delta_{L+1}$, and the coupling constant is set to $\kappa = \kappa_{\mathcal{S}}$. The one particle Hamiltonian of the coupled system is h_{crystal}.

We emphasize that the crystallization of the sample is specified by the pair $(\mathcal{S}, \kappa_{\mathcal{S}})$ and not by $\mathcal{S}$ alone.

The Bloch-Floquet decomposition of h_{crystal} reads

$$\ell^2(\mathbb{Z}) = \int_{\mathfrak{B}_L}^{\oplus} \mathfrak{h}_{\mathcal{S}} \, \mathrm{d}k, \qquad h_{\text{crystal}} = \int_{\mathfrak{B}_L}^{\oplus} h(k) \, \mathrm{d}k,$$

where $\mathfrak{B}_L = [-\pi/L, \pi/L]$ is the first Brillouin zone of the crystal and $h(k)$ is the self-adjoint operator on $\mathfrak{h}_{\mathcal{S}}$ obtained from (1.1) by replacing Dirichlet by Bloch boundary conditions

$$u(0) = \mathrm{e}^{-\mathrm{i}kL} u(L), \qquad u(L+1) = \mathrm{e}^{\mathrm{i}kL} u(1).$$

The spectrum of $h(k)$ consists of L eigenvalues $\varepsilon_1(k) \leq \cdots \leq \varepsilon_L(k)$ which are even functions of k, real analytic and strictly monotone on $]0, \pi/L[$. Moreover

$$\varepsilon_L(0) > \varepsilon_L(\pi/L) \geq \varepsilon_{L-1}(\pi/L) > \varepsilon_{L-1}(0) \geq \varepsilon_{L-2}(0) > \cdots$$

Thus, the spectrum of h_{crystal} is

$$\mathrm{sp}(h_{\text{crystal}}) = \bigcup_{k \in \mathcal{B}_L} \mathrm{sp}(h(k)) = \bigcup_{j=1}^{L} B_j,$$

where B_j is a closed interval with boundary points $\varepsilon_j(0)$ and $\varepsilon_j(\pi/L)$ (see Theorem 5.3.4 in [Si] and Figure 1).

For simplicity, suppose that the reservoirs are at zero temperature, i.e., $\beta_l = \beta_r = \infty$, and assume that $\mu_l < \mu_r$. In this case the function Δ_r is the characteristic function of the interval $[\mu_l, \mu_r]$ and the Landauer-Büttiker formula for the steady charge current out of the right reservoir becomes

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

Since the transmittance of a unit cell in a perfect crystal is the characteristic function of its spectrum, we get

$$\omega_+(\mathcal{J}_r) = \frac{1}{2\pi} |\mathrm{sp}(h_{\text{crystal}}) \cap [\mu_l, \mu_r]|,$$

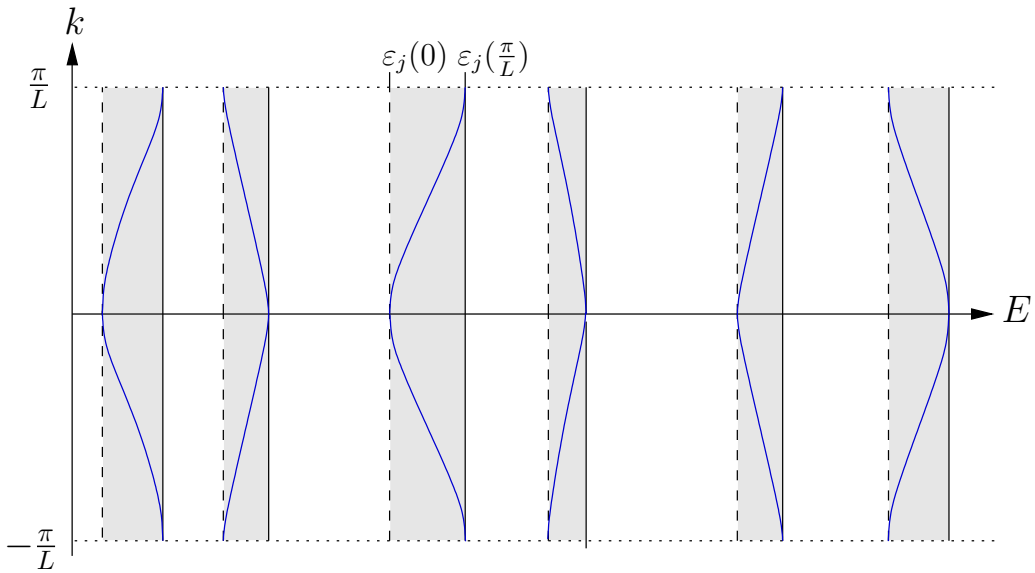

Figure 1: Eigenvalues of $h(k)$ and the band spectrum of h_{crystal}.

from which we infer that the mean conductance of the sample on the energy window $I = [\mu_l, \mu_r]$ is given by

$$g(I) = \frac{1}{2\pi} \frac{|\text{sp}(h_{\text{crystal}}) \cap I|}{|I|}.$$

We shall now argue that this expression can be interpreted as the Thouless conductance associated to the energy window I. In order for the level spacing ΔE to be well defined, the interval I should contain several bands B_j of h_{crystal}. The energy uncertainty within a single band $B_j \subset I$ is of the order of the band width $|B_j| = |\varepsilon_j(\pi/L) - \varepsilon_j(0)|$ which coincides with the variation of the eigenvalue $\varepsilon_j(k)$ as the Bloch boundary condition changes from periodic to anti-periodic (see Figure 2). A rough but convenient estimate of the energy uncertainty within the window I is given by the arithmetic mean

$$\delta E \sim \frac{\sum_{B_j \subset I} |B_j|}{\sum_{B_j \subset I} 1} \sim \frac{|\text{sp}(h_{\text{crystal}}) \cap I|}{\sum_{B_j \subset I} 1}.$$

On the other hand, the mean level spacing within I is given by

$$\Delta E \sim \frac{|I|}{\sum_{B_j \subset I} 1},$$

and the Thouless conductance becomes

$$g_{\text{Th}} \sim \frac{\delta E}{\Delta E} \sim \frac{|\text{sp}(h_{\text{crystal}}) \cap I|}{|I|}.$$

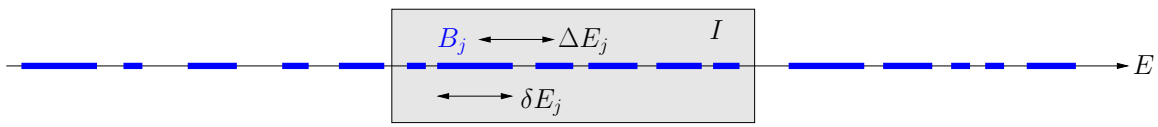

Figure 2: Energy uncertainty δE_j and level spacing ΔE_j for the j-th band in the window I.

According to the previous arguments, we shall *define* the Thouless conductance of the pair $(\mathcal{S}, \kappa_{\mathcal{S}})$ for the energy window $I \subset \mathbb{R}$ by

$$g_{\mathrm{Th}}(I) = \frac{1}{2\pi} \frac{|\mathrm{sp}(h_{\mathrm{crystal}}) \cap I|}{|I|}, \tag{1.9}$$

where h_{crystal} is the periodization of $h_{\mathcal{S}}$ with $J_L = \kappa_{\mathcal{S}}$.

Note that if $\kappa_{\mathcal{S}} = 0$, then $\mathrm{sp}(h_{\mathrm{crystal}}) = \mathrm{sp}(h_{\mathcal{S}})$ and $g_{\mathrm{Th}}(I) = 0$ for all intervals I. More generally, the width of the L Bloch bands satisfies $|B_j| = \mathcal{O}(\kappa_{\mathcal{S}})$ as $\kappa_{\mathcal{S}} \to 0$, and

$$g_{\mathrm{Th}}(I) = \mathcal{O}(\kappa_{\mathcal{S}})$$

in this limit.

2 The crystalline limit

To further elaborate on the connection between Thouless conductance and the Landauer-Büttiker formula, we shall now consider the approximation of h_{crystal} by finite repetitions of the sample $\mathcal{S}$ connected to arbitrary reservoirs.

Let h_{crystal} be as in the previous section. Given a positive integer N, let $h_{\mathcal{S}}^{(N)}$ be the restriction of h_{crystal} to the finite lattice $Z_{NL} = [1, NL] \cap \mathbb{Z}$ with Dirichlet boundary condition. Hence $h_{\mathcal{S}}^{(N)}$ is a Jacobi matrix acting on $\mathfrak{h}_{\mathcal{S}}^{(N)} = \ell^2(Z_{NL})$ whose Jacobi parameters satisfy

$$J_{x+nL} = J_x, \qquad \lambda_{x+nL} = \lambda_x, \qquad (x \in Z_L, n = 0, 1, \ldots, N-1),$$

where $\{J_x\}_{1 \le x < L}$ and $\{\lambda_x\}_{1 \le x \le L}$ are the Jacobi parameters of the original sample Hamiltonian $h_{\mathcal{S}}$ and $J_L = \kappa_{\mathcal{S}}$. The pairs $(\mathfrak{h}_{\mathcal{S}}^{(N)}, h_{\mathcal{S}}^{(N)})$ define a sequence of sample systems which are coupled to the reservoirs $\mathcal{R}_{l/r}$ as in Section 1.1. The reservoirs' single particle Hilbert spaces and Hamiltonains $(\mathfrak{h}_{l/r}, h_{l/r})$, the vectors $\chi_{l/r}$, and the coupling strength κ do not depend on N, and one takes $\psi_l = \delta_1$, $\psi_r = \delta_{NL}$. We assume that the one-particle Hamiltonian $h^{(N)}$ of the coupled systems satisfies Assumption **A** for all N [4] and we denote by $\omega_+^{(N)}$, $\Phi_{l/r}^{(N)}$, $\mathcal{I}_{l/r}^{(N)}$, $\mathcal{J}^{(N)}$ the respective NESS and flux observables. We are interested in the large N limit of the charge, energy and entropy steady currents (see Figure 3).

[4] Besides the crystaline ones, see Section 1.2.2, a concrete example of reservoirs where this is the case is $\mathfrak{h}_{l/r} = \ell^2(\mathbb{Z}_+)$, $h_{l/r} = -k\Delta$, $k > 0$. For other examples and general results regarding this point we refer the reader to [GJW].

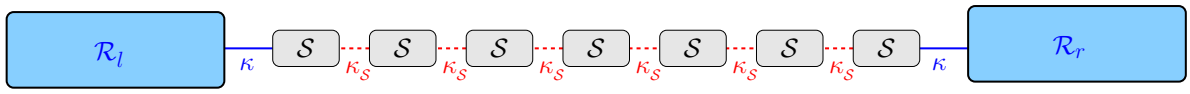

Figure 3: The EBBM described by the Hamiltonian $h^{(N)}$ for $N = 7$.

Let $h^{(l)}_{\text{crystal}}$ and $h^{(r)}_{\text{crystal}}$ be the restrictions of h_{crystal} to $\ell^2((-\infty, 0] \cap \mathbb{Z})$ and $\ell^2([1, \infty) \cap \mathbb{Z})$ with Dirichlet boundary conditions. Denote by

$$\begin{aligned} m_l(E) &= \langle \delta_0, (h^{(l)}_{\text{crystal}} - E - \mathrm{i}0)^{-1}\delta_0\rangle, \\ m_r(E) &= \langle \delta_1, (h^{(r)}_{\text{crystal}} - E - \mathrm{i}0)^{-1}\delta_1\rangle, \end{aligned} \tag{2.1}$$

the respective Weyl m-functions. One easily shows that $\operatorname{Im} m_{l/r}(E) > 0$ for Lebesgue a.e. $E \in \operatorname{sp}(h_{\text{crystal}})$. We set $\mathcal{T}_\infty(E) = 0$ for $E \in \mathbb{R} \setminus (\operatorname{sp}(h_{\text{crystal}}) \cap \Sigma_l \cap \Sigma_r)$ and

$$\mathcal{T}_\infty(E) = \left[1 + \frac{1}{4}\left(\frac{|\kappa_{\mathcal{S}}^2 m_r(E) - \kappa^2 F_r(E)|^2}{\operatorname{Im}(\kappa_{\mathcal{S}}^2 m_r(E))\operatorname{Im}(\kappa^2 F_r(E))} + \frac{|\kappa_{\mathcal{S}}^2 m_l(E) - \kappa^2 F_l(E)|^2}{\operatorname{Im}(\kappa_{\mathcal{S}}^2 m_l(E))\operatorname{Im}(\kappa^2 F_l(E))}\right)\right]^{-1} \tag{2.2}$$

for $E \in \operatorname{sp}(h_{\text{crystal}}) \cap \Sigma_l \cap \Sigma_r$. Obviously, $0 \le \mathcal{T}_\infty(E) \le 1$ for Lebesgue a.e. $E \in \mathbb{R}$.

Let

$$\mathcal{T}_N(E) = 4\kappa^4 |\langle \psi_l, (h^{(N)} - E - \mathrm{i}0)^{-1}\psi_r\rangle|^2 \operatorname{Im} F_l(E) \operatorname{Im} F_r(E),$$

be the transmittance of the N-fold repeated pair $(\mathcal{S}, \kappa_{\mathcal{S}})$. Our main technical result is:

Theorem 2.1 *For any $f \in L^1(\mathbb{R})$ one has*

$$\lim_{N\to\infty} \int \mathcal{T}_N(E) f(E)\,\mathrm{d}E = \int \mathcal{T}_\infty(E) f(E)\,\mathrm{d}E. \tag{2.3}$$

The proof of this theorem is given in Section 3. As an immediate consequence, one has

Theorem 2.2

$$\begin{aligned} \langle \Phi_{l/r}\rangle_\infty &= \lim_{N\to\infty} \omega_+^{(N)}(\Phi^{(N)}_{l/r}) = \frac{1}{2\pi}\int_{\operatorname{sp}(h_{\text{crystal}})} \mathcal{T}_\infty(E) E \Delta_{l/r}(E)\,\mathrm{d}E, \\ \langle \mathcal{I}_{l/r}\rangle_\infty &= \lim_{N\to\infty} \omega_+^{(N)}(\mathcal{I}^{(N)}_{l/r}) = \frac{1}{2\pi}\int_{\operatorname{sp}(h_{\text{crystal}})} \mathcal{T}_\infty(E) \Delta_{l/r}(E)\,\mathrm{d}E, \\ \langle \mathcal{J}\rangle_\infty &= \lim_{N\to\infty} \omega_+^{(N)}(\mathcal{J}^{(N)}) = \frac{1}{2\pi}\int_{\operatorname{sp}(h_{\text{crystal}})} \mathcal{T}_\infty(E) \varsigma(E)\,\mathrm{d}E. \end{aligned} \tag{2.4}$$

Obviously, the conservation laws

$$\langle \Phi_l \rangle_\infty + \langle \Phi_r \rangle_\infty = 0,$$

$$\langle \mathcal{I}_l \rangle_\infty + \langle \mathcal{I}_r \rangle_\infty = 0,$$

hold, as well as the entropy balance relation

$$\langle \mathcal{J} \rangle_\infty = -\beta_l(\langle \Phi_l \rangle_\infty - \mu_l \langle \mathcal{I}_l \rangle_\infty) - \beta_r(\langle \Phi_r \rangle_\infty - \mu_r \langle \mathcal{I}_r \rangle_\infty).$$

2.1 Thouless conductance revisited

Given a finite sample described by $\mathfrak{h}_\mathcal{S}$, $h_\mathcal{S}$, $\kappa_\mathcal{S}$ and its periodization h_{crystal}, the Thouless currents associated to chemical potentials $\mu_{l/r}$ and inverse temperatures $\beta_{l/r}$ are defined by setting $\mathcal{T}_\infty(E) = 1$ in the formulas (2.4), i.e., by assuming that the transport between the reservoirs is reflectionless. The Thouless current formulas are:

$$\begin{aligned} \langle \Phi_{l/r} \rangle_{\text{Th}} &= \frac{1}{2\pi} \int_{\text{sp}(h_{\text{crystal}})} E \Delta_{l/r}(E) \mathrm{d}E, \\ \langle \mathcal{I}_{l/r} \rangle_{\text{Th}} &= \frac{1}{2\pi} \int_{\text{sp}(h_{\text{crystal}})} \Delta_{l/r}(E) \mathrm{d}E, \\ \langle \mathcal{J} \rangle_{\text{Th}} &= \frac{1}{2\pi} \int_{\text{sp}(h_{\text{crystal}})} \varsigma(E) \mathrm{d}E. \end{aligned} \tag{2.5}$$

One has again the conservation laws

$$\langle \Phi_l \rangle_{\text{Th}} + \langle \Phi_r \rangle_{\text{Th}} = 0,$$

$$\langle \mathcal{I}_l \rangle_{\text{Th}} + \langle \mathcal{I}_r \rangle_{\text{Th}} = 0,$$

and

$$\langle \mathcal{J} \rangle_{\text{Th}} = -\beta_l(\langle \Phi_l \rangle_{\text{Th}} - \mu_l \langle \mathcal{I}_l \rangle_{\text{Th}}) - \beta_r(\langle \Phi_r \rangle_{\text{Th}} - \mu_r \langle \mathcal{I}_r \rangle_{\text{Th}}).$$

Recall the definition of crystalline EBBM given in Section 1.2.2. The following theorem is a direct consequence of the definition of Thouless currents (2.5) and of Theorem 2.2.

Theorem 2.3 (1)

$$\langle \mathcal{J} \rangle_{\text{Th}} = \sup \langle \mathcal{J} \rangle_\infty,$$

where the supremum is taken over all realizations of the reservoirs. Moreover, this supremum is achieved if the EBBM is crystalline.

(2) *If* $\mu_l = \mu_r = \mu$, $\mu \leq \inf \mathrm{sp}(h_{\mathrm{crystal}})$, *and* $\beta_l > \beta_r$, *then*

$$\langle \Phi_r \rangle_{\mathrm{Th}} = \sup \, \langle \Phi_r \rangle_\infty,$$

and the supremum is achieved if the EBBM is crystalline. If $\beta_l < \beta_r$, *then this result holds for* $\langle \Phi_l \rangle$. *If* $\mu \geq \sup \mathrm{sp}(h_{\mathrm{crystal}})$, *the same results hold with exchange of* l *and* r.

(3) *If* $\beta_l = \beta_r$ *and* $\mu_l < \mu_r$, *then*

$$\langle \mathcal{I}_r \rangle_{\mathrm{Th}} = \sup \, \langle \mathcal{I}_r \rangle_\infty,$$

and the supremum is achieved if the EBBM is crystalline. If $\mu_l > \mu_r$, *then this result holds for* $\langle \mathcal{I}_l \rangle$.

Remark 1. All suprema in the previous theorem are achieved iff the transport between the reservoirs is reflectionless, that is, iff $\mathcal{T}_\infty(E) = 1$ for Lebesgue a.e. $E \in \mathrm{sp}(h_{\mathrm{crystal}})$. The crystalline EBBM provide such reservoirs. To elucidate this point further, note that $\mathcal{T}_\infty(E) = 1$ for Lebesgue a.e. $E \in \mathrm{sp}(h_{\mathrm{crystal}})$ iff $\sigma(h_{\mathrm{crystal}}) \subset \Sigma_l \cap \Sigma_r$ and

$$\kappa_{\mathcal{S}}^2 m_{r/l}(E) = \kappa^2 F_{r/l}(E),$$

for Lebesgue a.e. $E \in \mathrm{sp}(h_{\mathrm{crystal}})$. Since $\mathrm{sp}(h_{\mathrm{crystal}})$ has positive Lebesgue measure, the theory of boundary values of analytic functions (see [Ja] or any book on harmonic analysis) yields that for any $z = E + \mathrm{i}\epsilon$ with $\epsilon > 0$,

$$\kappa_{\mathcal{S}}^2 \langle \delta_0, (h_{\mathrm{crystal}}^{(l)} - z)^{-1} \delta_0 \rangle = \kappa^2 \langle \chi_l, (h_l - z)^{-1} \chi_l \rangle,$$

$$\kappa_{\mathcal{S}}^2 \langle \delta_1, (h_{\mathrm{crystal}}^{(r)} - z)^{-1} \delta_1 \rangle = \kappa^2 \langle \chi_r, (h_r - z)^{-1} \chi_r \rangle.$$

These relations imply

$$\kappa_{\mathcal{S}}^2 \nu_{\mathrm{crystal}}^{(l/r)} = \kappa^2 \nu_{l/r},$$

where $\nu_{\mathrm{crystal}}^{(l/r)}$ is the spectral measure of $h_{\mathrm{crystal}}^{(l/r)}$ associated to δ_0/δ_1. Since $\nu_{\mathrm{crystal}}^{(l/r)}$ and $\nu_{l/r}$ are probability measures, we conclude that $\kappa_{\mathcal{S}}^2 = \kappa^2$ and $\nu_{\mathrm{crystal}}^{(l/r)} = \nu_{l/r}$. Thus, the transport between the reservoirs is reflectionless iff $\kappa^2 = \kappa_{\mathcal{S}}^2$ and $h_{r/l}$ is unitarily equivalent to $h_{\mathrm{crystal}}^{(r/l)}$. In other words, all suprema in the previous theorem are achieved iff the EBBM is unitarily equivalent to a crystalline EBMM up to (for the transport purposes) irrelevant choice of the sign of κ.

Remark 2. Part (2) holds whenever $E\Delta_{l/r}(E)$ has a definite sign on $\mathrm{sp}(h_{\mathrm{crystal}})$ and, similarly, Part (3) holds whenever $\Delta_{l/r}(E)$ has a definite sign on $\mathrm{sp}(h_{\mathrm{crystal}})$. In the lack of a definite sign one cannot expect a variational characterization of Thouless currents in terms of the crystalline Landauer-Büttiker currents. Note that

$$\Delta_{l/r}(E) = \frac{\sinh((\zeta_{r/l}(E) - \zeta_{l/r}(E))/2)}{2\cosh(\zeta_l(E)/2)\cosh(\zeta_r(E)/2)},$$

so that the sign of $\Delta_{l/r}(E)$ is the same as the sign of

$$\zeta_{r/l}(E) - \zeta_{l/r}(E) = (\beta_{r/l} - \beta_{l/r})E - (\beta_{r/l}\mu_{l/r} - \beta_{l/r}\mu_{l/r}).$$

In the non-trivial case $\beta_l \neq \beta_r$, $\Delta_{l/r}(E)$ changes the sign at precisely one point

$$E_c = \frac{\beta_{r/l}\mu_{l/r} - \beta_{l/r}\mu_{l/r}}{\beta_{r/l} - \beta_{l/r}}.$$

If additional information about $\mathrm{sp}(h_{\mathrm{crystal}})$ is available, the above fact can be used to obtain further relations between the crystalline Landauer-Büttiker currents (2.4) and Thouless currents (2.5).

Remark 3. If $\beta_l = \beta_r = \infty$, $\mu_l < \mu_r$, and $I = [\mu_l, \mu_r]$, then

$$\langle \Phi_r \rangle_{\mathrm{Th}} = \frac{1}{2\pi} \int_{\mathrm{sp}(h_{\mathrm{crystal}}) \cap I} E \mathrm{d}E,$$

$$\langle \mathcal{I}_r \rangle_{\mathrm{Th}} = \frac{1}{2\pi} |\mathrm{sp}(h_{\mathrm{crystal}}) \cap I|.$$

Thus, the Thouless formula (1.9) indeed describes the maximal conductance at zero temperature for the given potential interval I:

$$g_{\mathrm{Th}}(I) = \frac{\langle \mathcal{I}_r \rangle_{\mathrm{Th}}}{\mu_r - \mu_l} = \sup \frac{\langle \mathcal{I}_r \rangle_{\infty}}{\mu_r - \mu_l}.$$

Remark 4. Since the crystalline Landauer-Büttiker formulas (2.4) are derived from the first principles of quantum statistical mechanics, Theorem 2.3 can be considered a rigorous quantum statistical derivation of the Thouless energy formula. This derivation also identifies the heuristic notion of "optimal feeding" of electrons with reflectionless transport between the reservoirs.

3 Proof of Theorem 2.1

3.1 Sample transmittance and Green matrix

We first connect the transmittance (1.2) to the sample's Green function. Recall that $F_{l/r}$ are defined in (1.3) and denote by $F(E)$ the 2×2 diagonal matrix with entries $F_l(E)$ and $F_r(E)$. We also introduce the 2×2 Green matrices $G_{\mathcal{S}}^{(N)}(z)$ and $G^{(N)}(z)$ with entries

$$G_{\mathcal{S},ab}^{(N)}(z) = \langle \psi_a, (h_{\mathcal{S}}^{(N)} - z)^{-1} \psi_b \rangle,$$

$$G_{ab}^{(N)}(z) = \langle \psi_a, (h^{(N)} - z)^{-1} \psi_b \rangle,$$

where $a, b \in \{l, r\}$ (recall that $\psi_l = \delta_1$ and $\psi_r = \delta_{NL}$). As usual, we write $G_{ab}^{(N)}(E) = G_{ab}^{(N)}(E + \mathrm{i}0)$.

The full Green matrix $G^{(N)}$ and the sample Green matrix $G_{\mathcal{S}}^{(N)}$ are related by (see Lemma 2.1 in [BJP])

$$G_{\mathcal{S}}^{(N)}(E) = (I - \kappa^2 G_{\mathcal{S}}^{(N)}(E) F(E)) G^{(N)}(E),$$

from which we deduce

$$G_{lr}^{(N)}(E) = \frac{G_{\mathcal{S},lr}^{(N)}(E)}{\det(I - \kappa^2 G_{\mathcal{S}}^{(N)}(E) F(E))}. \tag{3.1}$$

Combined with (1.2) and (1.6) this allows us the expression of the transmittance of the sample and hence the steady currents in terms of the Green matrix $G_{\mathcal{S}}^{(N)}$.

3.2 Green and transfer matrix

Our next step is to relate the sample's Green matrix to the transfer matrix of the periodic Jacobi matrix h_{crystal}.

Following [Si] the transfer matrix at energy E is defined by

$$T_n(E) = A_n(E) \cdots A_1(E),$$

where

$$A_x(E) = J_x^{-1} \begin{bmatrix} E - \lambda_x & -1 \\ J_x^2 & 0 \end{bmatrix}.$$

Note that $\det A_x(E) = 1$ for any x and hence $\det T_n(E) = 1$ as well. A function u satisfies the finite difference equation $h_{\text{crystal}} u = Eu$ if and only if for any x one has

$$A_x \begin{bmatrix} u(x) \\ J_{x-1} u(x-1) \end{bmatrix} = \begin{bmatrix} u(x+1) \\ J_x u(x) \end{bmatrix}.$$

Lemma 3.1 *For any $x, y, u, v \in \mathbb{C}$ one has*

$$G_{\mathcal{S}}^{(N)}(E) \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} u \\ v \end{bmatrix} \Longleftrightarrow T_{NL}(E) \begin{bmatrix} u \\ -x \end{bmatrix} = \begin{bmatrix} -\kappa_{\mathcal{S}}^{-1} y \\ \kappa_{\mathcal{S}} v \end{bmatrix}.$$

In other words, the matrix $P : (x, y, u, v) \mapsto (u, -x, -\kappa_{\mathcal{S}}^{-1} y, \kappa_{\mathcal{S}} v)$ maps the graph of $G_{\mathcal{S}}^{(N)}(E)$ to that of $T_{NL}(E)$.

Remark. This lemma is a slight generalization of Lemma 2.2 in [BJP]. We include the proof for the reader convenience.

Proof. Fix N and $E \in \mathbb{R} \setminus \mathrm{sp}(h_{\mathcal{S}}^{(N)})$. For $f \in \ell^2(Z_{NL})$, the function

$$u(x) = \langle \delta_x, (h_{\mathcal{S}}^{(N)} - E)^{-1} f \rangle$$

satisfies the finite difference equation

$$(h_{\text{crystal}} - E)u = f, \tag{3.2}$$

with boundary conditions $u(0) = u(NL+1) = 0$. Using the transfer matrix

$$T(x,y) = A_x A_{x-1} \cdots A_{y+1},$$

the solution of the initial value problem for (3.2) can be written as

$$\begin{bmatrix} u(x+1) \\ J_x u(x) \end{bmatrix} = T(x,0) \begin{bmatrix} u(1) \\ J_0 u(0) \end{bmatrix} - \sum_{y=1}^{x} T(x,y-1) \begin{bmatrix} 0 \\ f(y) \end{bmatrix}.$$

Setting $x = NL$ and taking the boundary conditions and $J_{NL} = J_0 = \kappa_{\mathcal{S}}$ into account yields

$$\begin{bmatrix} 0 \\ \kappa_{\mathcal{S}} u(NL) \end{bmatrix} = T_{NL}(E) \begin{bmatrix} u(1) \\ 0 \end{bmatrix} - \sum_{y=1}^{NL} T(NL,y-1) \begin{bmatrix} 0 \\ f(y) \end{bmatrix},$$

which is an equation for the unknown $u(1)$ and $u(NL)$. Setting $f = \delta_1$ and $f = \delta_{NL}$, we obtain the following equations for the entries of the matrix $G_{\mathcal{S}}^{(N)}(E)$:

$$T_{NL}(E) \begin{bmatrix} G_{\mathcal{S},ll}^{(N)}(E) \\ -1 \end{bmatrix} = \begin{bmatrix} 0 \\ \kappa_{\mathcal{S}} G_{\mathcal{S},rl}^{(N)}(E) \end{bmatrix},$$

$$T_{NL}(E) \begin{bmatrix} G_{\mathcal{S},lr}^{(N)}(E) \\ 0 \end{bmatrix} = \begin{bmatrix} -\kappa_{\mathcal{S}}^{-1} \\ \kappa_{\mathcal{S}} G_{\mathcal{S},rr}^{(N)}(E) \end{bmatrix}.$$

Thus, the two linearly independent vectors

$$\left\{ [G_{\mathcal{S},ll}^{(N)}(E), -1, 0, \kappa_{\mathcal{S}} G_{\mathcal{S},rl}^{(N)}(E)]^T, [G_{\mathcal{S},lr}^{(N)}(E), 0, -\kappa_{\mathcal{S}}^{-1}, \kappa_{\mathcal{S}} G_{\mathcal{S},rr}^{(N)}(E)]^T \right\},$$

span the graph of $T_{NL}(E)$. One easily checks that they are the images by the matrix P of the two vectors $[1, 0, G_{\mathcal{S},ll}^{(N)}(E), G_{\mathcal{S},rl}^{(N)}(E)]^T$ and $[0, 1, G_{\mathcal{S},lr}^{(N)}(E), G_{\mathcal{S},rr}^{(N)}(E)]^T$ which span the graph of $G_{\mathcal{S}}^{(N)}(E)$. □

3.3 Transfer matrix eigenvalues and eigenfunctions

Since the Jacobi matrix h_{crystal} is periodic, one has $T_{NL}(E) = T_L(E)^N$ for any N. The eigenvalues and eigenvectors of the one-period transfer matrix $T_L(E)$ will thus play an important role. Since $\det T_L(E) = 1$, we may write its eigenvalues as $\alpha(E)$ and $\alpha(E)^{-1}$. It is a standard result (see, e.g., [RS4, Si]) that these eigenvalues are either complex conjugated (and hence of modulus 1) or real. The first case occurs iff $|\operatorname{tr} T_L(E)| \leq 2$ which is in turn equivalent to $E \in \operatorname{sp}(h_{\text{crystal}})$. We denote by

$$\Psi_\pm(E) = \begin{bmatrix} \phi_\pm(E) \\ \kappa_{\mathcal{S}}\psi_\pm(E) \end{bmatrix}$$

an eigenvector of $T_L(E)$ associated to its eigenvalue $\alpha(E)^{\pm 1}$ with the following conventions:

(N1) When $E \notin \operatorname{sp}(h_{\text{crystal}})$ we chose $|\alpha(E)|^{-1} < 1 < |\alpha(E)|$ and real eigenvectors.

(N2) When $E \in \operatorname{sp}(h_{\text{crystal}})$ we chose $\Psi_-(E) = \overline{\Psi_+(E)}$. Since the two eigenvectors are linearly independent, they can be normalized by $\phi_\pm(E) = 1$, which further implies $\operatorname{Im}\psi_\pm(E) \neq 0$. We then select $\alpha(E)$ such that $\operatorname{Im}\psi_+(E) > 0$.

Using Lemma 3.1 and $T_{NL}(E) = T_L(E)^N$, we get

$$G_{\mathcal{S}}^{(N)}(E) = \frac{-\kappa_{\mathcal{S}}^{-1}}{D_N(E)} \begin{bmatrix} \phi_+(E)\phi_-(E)(\alpha(E)^N - \alpha(E)^{-N}) & \phi_+(E)\psi_-(E) - \phi_-(E)\psi_+(E) \\ \phi_+(E)\psi_-(E) - \phi_-(E)\psi_+(E) & \psi_+(E)\psi_-(E)(\alpha(E)^N - \alpha(E)^{-N}) \end{bmatrix}$$

where

$$D_N(E) = \alpha(E)^N\phi_+(E)\psi_-(E) - \alpha(E)^{-N}\phi_-(E)\psi_+(E).$$

An elementary calculation yields

$$\det(I - \kappa^2 G_{\mathcal{S}}^{(N)}(E)F(E)) = \frac{\alpha(E)^N\widetilde{\phi}_+(E)\widetilde{\psi}_-(E) - \alpha(E)^{-N}\widetilde{\phi}_-(E)\widetilde{\psi}_+(E)}{\alpha(E)^N\phi_+(E)\psi_-(E) - \alpha(E)^{-N}\phi_-(E)\psi_+(E)},$$

where

$$\widetilde{\psi}_\pm(E) = \psi_\pm(E) + \eta^2\kappa_{\mathcal{S}}\phi_\pm(E)F_l(E), \qquad \widetilde{\phi}_\pm(E) = \phi_\pm(E) + \eta^2\kappa_{\mathcal{S}}\psi_\pm(E)F_r(E), \tag{3.3}$$

and we have set

$$\eta = \frac{\kappa}{\kappa_{\mathcal{S}}}.$$

Inserting the last relations into (3.1) leads to the following expression for the off-diagonal element of the full Green matrix

$$G_{lr}^{(N)}(E) = -\kappa_{\mathcal{S}}^{-1}\frac{\phi_+(E)\psi_-(E) - \phi_-(E)\psi_+(E)}{\alpha(E)^N\widetilde{\phi}_+(E)\widetilde{\psi}_-(E) - \alpha(E)^{-N}\widetilde{\phi}_-(E)\widetilde{\psi}_+(E)}. \tag{3.4}$$

3.4 The large N limit

We proceed to evaluate the large N limit of $\mathcal{T}_N(E)$ in distributional sense.

We write the left hand side of (2.3) as $\mathcal{T}_{N,1}(f) + \mathcal{T}_{N,2}(f)$ with

$$\mathcal{T}_{N,1}(f) = \int_{\mathrm{sp}(h_{\mathrm{crystal}})\cap\Sigma_l\cap\Sigma_r} \mathcal{T}_N(E) f(E)\,\mathrm{d}E,$$

$$\mathcal{T}_{N,2}(f) = \int_{\mathbb{R}\setminus(\mathrm{sp}(h_{\mathrm{crystal}})\cap\Sigma_l\cap\Sigma_r)} \mathcal{T}_N(E) f(E)\,\mathrm{d}E.$$

To deal with $\mathcal{T}_{N,2}(f)$ we prove

Lemma 3.2 *For almost all $E \in \mathbb{R} \setminus (\mathrm{sp}(h_{\mathrm{crystal}}) \cap \Sigma_l \cap \Sigma_r)$ one has*

$$\lim_{N\to\infty} \mathcal{T}_N(E) = 0.$$

Proof. Combining (1.2) and (3.4), we get

$$\mathcal{T}_N(E) = 4\kappa^2\eta^2 \left| \frac{\phi_+(E)\psi_-(E) - \phi_-(E)\psi_+(E)}{\alpha(E)^N\widetilde{\phi}_+(E)\widetilde{\psi}_-(E) - \alpha(E)^{-N}\widetilde{\phi}_-(E)\widetilde{\psi}_+(E)} \right|^2 \mathrm{Im}\, F_l(E)\,\mathrm{Im}\, F_r(E).$$

It follows from (1.4) that $\mathcal{T}_N(E) = 0$ for almost all $E \in \mathbb{R} \setminus (\Sigma_l \cap \Sigma_r)$ and all N. Thus, it suffices to consider $E \in (\Sigma_l \cap \Sigma_r) \setminus \mathrm{sp}(h_{\mathrm{crystal}})$.

For such E, the eigenvectors $\Psi_\pm(E)$ are real and $|\alpha(E)| > 1$ by Condition (N1). Moreover, $\mathrm{Im}\, F_{l/r}(E) > 0$ by (1.5). We claim that this implies $\widetilde{\phi}_+(E)\widetilde{\psi}_-(E) \neq 0$ from which the result clearly follows. To prove this claim, we argue by contradiction. Assume that $\widetilde{\phi}_+(E) = 0$ (the case $\widetilde{\psi}_-(E) = 0$ is similar). It follows from (3.3) that

$$\mathrm{Im}\,\widetilde{\phi}_+(E) = \eta^2\kappa_{\mathcal{S}}\psi_+(E)\mathrm{Im}\, F_r(E) = 0,$$

and hence $\psi_+(E) = 0$. Using (3.3) again we get $\phi_+(E) = \widetilde{\phi}_+(E) = 0$. We conclude that $\Psi_+(E) = 0$, a contradiction. □

Since $0 \leq \mathcal{T}_N(E) \leq 1$ and $f \in L^1(\mathbb{R})$, Lemma 3.2 and the dominated convergence theorem yield that $\mathcal{T}_{N,2}(f) \to 0$ as $N \to \infty$. It thus remains to analyze $\mathcal{T}_{N,1}(f)$. To this end, we relate the eigenvectors of T_L to the Weyl m-functions (2.1).

Lemma 3.3 *For any $E \in \mathrm{sp}(h_{\mathrm{crystal}})$, we have*

$$\psi_+(E) = -\frac{1}{\kappa_{\mathcal{S}} m_r(E)}, \qquad \psi_-(E) = -\kappa_{\mathcal{S}} m_l(E).$$

Proof. Let us write the one-period transfer matrix as

$$T_L(E) = \begin{bmatrix} a(E) & b(E) \\ c(E) & d(E) \end{bmatrix}. \tag{3.5}$$

Since $\det T_L(E) = 1$, we can write the discriminant of the quadratic equation

$$c(E)z^2 + (a(E) - d(E))z - b(E) = 0, \tag{3.6}$$

as $(\operatorname{tr} T_L(E))^2 - 4$, which is negative for $E \in \operatorname{sp}(h_{\text{crystal}})$. Thus, (3.6) has two complex conjugate solutions. The solution with positive imaginary part is $m_r(E)$ and the other one is $1/\kappa_{\mathcal{S}}^2 m_l(E)$. We refer the reader to Section 5.2 in [Si] for a proof of these facts.

Using the representation (3.5) and taking Condition (N2) into account, one easily shows that the eigenvalues and eigenvectors of $T_L(E)$ are determined by $\alpha(E) = \mathrm{e}^{\mathrm{i}\theta(E)}$ and

$$\kappa_{\mathcal{S}}\psi_{\pm}(E) = \frac{1}{b(E)}\left(\mathrm{e}^{\pm\mathrm{i}\theta(E)} - a(E)\right) = \frac{1}{b(E)}\left(\frac{d(E) - a(E)}{2} \pm \mathrm{i}\sin\theta(E)\right), \tag{3.7}$$

where $\theta(E) \in]-\pi, \pi[$ is defined by

$$\cos\theta(E) = \frac{1}{2}\operatorname{tr} T_L(E), \qquad \operatorname{sign}(\theta(E)) = \operatorname{sign}(b(E)). \tag{3.8}$$

Note that the product of the two solutions of (3.6) is

$$-\frac{b(E)}{c(E)} = \frac{m_r(E)}{\kappa_{\mathcal{S}}^2 m_l(E)} = |m_r(E)|^2 > 0, \tag{3.9}$$

so that $b(E)$ and $c(E)$ have opposite signs. It follows that the solutions of (3.6) are

$$m_r(E) = \frac{1}{c(E)}\left(\frac{d(E) - a(E)}{2} - \mathrm{i}\sin\theta(E)\right),$$

$$\frac{1}{\kappa_{\mathcal{S}}^2 m_l(E)} = \frac{1}{c(E)}\left(\frac{d(E) - a(E)}{2} + \mathrm{i}\sin\theta(E)\right).$$

Comparing these relations with (3.7) and using (3.9) yield the result. □

To formulate our next result, let the real functions $r(E) \geq 0$ and $\vartheta(E)$ be defined by the following polar decomposition

$$\frac{m_l(E) - \eta^2 F_l(E)}{\overline{m}_l(E) - \eta^2 F_l(E)}\,\frac{m_r(E) - \eta^2 F_r(E)}{\overline{m}_r(E) - \eta^2 F_r(E)}\,\frac{\overline{m}_r(E)}{m_r(E)} = r(E)\mathrm{e}^{\mathrm{i}\vartheta(E)}. \tag{3.10}$$

Lemma 3.4 *Let $I \subset \mathrm{sp}(h_{\mathrm{crystal}}) \cap \Sigma_l \cap \Sigma_r$. If there exists $\delta < 1$ such that $r(E) \leq \delta$ for almost all $E \in I$, then*

$$\lim_{N\to\infty} \int_I \mathcal{T}_N(E) f(E)\,\mathrm{d}E = \int_I \mathcal{T}_\infty(E) f(E)\,\mathrm{d}E,$$

for any $f \in L^1(\mathbb{R})$.

Proof. Combining Lemma 3.3 with (1.2) and (3.4) we can write the transmittance of the N-fold repeated sample as

$$\mathcal{T}_N(E) = \frac{16\eta^4 \mathrm{Im}\, m_r(E)\, \mathrm{Im}\, m_l(E)}{|\overline{m}_r(E) - \eta^2 F_r(E)|^2 |\overline{m}_l(E) - \eta^2 F_l(E)|^2} \frac{\mathrm{Im}\ F_l(E)\, \mathrm{Im}\ F_r(E)}{|1 - r(E)\mathrm{e}^{\mathrm{i}(2N\theta(E)+\vartheta(E))}|^2}, \tag{3.11}$$

where $\theta(E)$ is defined by (3.8). Expanding the right hand side of (3.11) in powers of $r(E)$, one obtains

$$\mathcal{T}_N(E) = \mathcal{T}_\infty(E) \sum_{k\in\mathbb{Z}} r(E)^{|k|} \mathrm{e}^{\mathrm{i}k(2N\theta(E)+\vartheta(E))},$$

where $\mathcal{T}_\infty(E)$ is given by (2.2). Since $r(E) \leq \delta < 1$ on I, this expansion is uniformly convergent for $E \in I$, and we have

$$\lim_{N\to\infty} \int_I \mathcal{T}_N(E) f(E)\,\mathrm{d}E = \lim_{N\to\infty} \sum_{k\in\mathbb{Z}} \int_I \mathcal{T}_\infty(E) r(E)^{|k|} \mathrm{e}^{\mathrm{i}k(2N\theta(E)+\vartheta(E))} f(E)\,\mathrm{d}E.$$

Since the function $\theta(E)$ is strictly monotone in each band of h_{crystal} (see, e.g., Sections 5.3-5.4 in [Si]), the Riemann-Lebesgue lemma yields the result. □

For $k > 0$, set

$$I_k = \{E \in \mathrm{sp}(h_{\mathrm{crystal}}) \cap \Sigma_l \cap \Sigma_r \,|\, \mathrm{Im}\, F_{l/r}(E) \geq 1/k \ \text{ and } \ |\mathrm{tr}\, T_L(E)| < 2 - 1/k\},$$

and $I'_k = (\mathrm{sp}(h_{\mathrm{crystal}}) \cap \Sigma_l \cap \Sigma_r) \setminus I_k$. Obviously,

$$\lim_{k\to\infty} |I'_k| = 0. \tag{3.12}$$

It follows from the proof of Lemma 3.3 that there is $\epsilon_k > 0$ such that $\mathrm{Im}\, m_{l/r}(E) \geq \epsilon_k$ for almost every $E \in I_k$. One easily concludes that there exists $\delta_k < 1$ such that

$$\left| \frac{m_{l/r}(E) - \eta^2 F_{l/r}(E)}{\overline{m}_{l/r}(E) - \eta^2 F_{l/r}(E)} \right| \leq \delta_k,$$

holds for almost every $E \in I_k$. Thus, for such E,

$$r(E) = \left| \frac{m_l(E) - \eta^2 F_l(E)}{\overline{m}_l(E) - \eta^2 F_l(E)} \right| \left| \frac{m_r(E) - \eta^2 F_r(E)}{\overline{m}_r(E) - \eta^2 F_r(E)} \right| \leq \delta_k^2 < 1.$$

Writing

$$\left|\mathcal{T}_{N,1}(f) - \int \mathcal{T}_\infty(E) f(E)\,\mathrm{d}E\right| \leq \left|\int_{I_k} (\mathcal{T}_N(E) - \mathcal{T}_\infty(E)) f(E)\,\mathrm{d}E\right| + \int_{I_k'} |(\mathcal{T}_N(E) - \mathcal{T}_\infty(E)) f(E)|\,\mathrm{d}E,$$

and applying Lemma 3.4 to I_k, we get

$$\limsup_{N\to\infty} \left|\mathcal{T}_{N,1}(f) - \int \mathcal{T}_\infty(E) f(E)\,\mathrm{d}E\right| \leq 2\int_{I_k'} |f(E)|\,\mathrm{d}E.$$

This estimate and (3.12) yield

$$\lim_{N\to\infty} \mathcal{T}_{N,1}(f) = \int \mathcal{T}_\infty(E) f(E)\,\mathrm{d}E$$

and Theorem 2.1 follows.

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