Landauer-Büttiker formula and Schrödinger conjecture

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Abstract. We study the entropy flux in the stationary state of a finite one-dimensional sample $\mathcal{S}$ connected at its left and right ends to two infinitely extended reservoirs $\mathcal{R}_{l/r}$ at distinct (inverse) temperatures $\beta_{l/r}$ and chemical potentials $\mu_{l/r}$. The sample is a free lattice Fermi gas confined to a box $[0, L]$ with energy operator $h_{\mathcal{S},L} = -\Delta + v$. The Landauer-Büttiker formula expresses the steady state entropy flux in the coupled system $\mathcal{R}_l + \mathcal{S} + \mathcal{R}_r$ in terms of scattering data. We study the behaviour of this steady state entropy flux in the limit $L \to \infty$ and relate persistence of transport to norm bounds on the transfer matrices of the limiting half-line Schrödinger operator $h_{\mathcal{S}}$.

1 Introduction

This paper is part of the program initiated in [AJPP1] and concerns transport in the so called electronic black box model. This model describes a sample $\mathcal{S}$ (e.g., a quantum dot or a more elaborate electronic device) coupled to several electronic reservoirs $\mathcal{R}_j$. These reservoirs are free Fermi gas in thermal equilibrium at given temperatures and chemical potentials. In the independent electron approximation, the coupled system $\mathcal{S}+\sum_j \mathcal{R}_j$ is a free Fermi gas with single particle Hamiltonian $h = h_0+h_{\mathrm{T}}$, where h_0 is the single particle Hamiltonian of the decoupled system and h_{T} is the tunneling Hamiltonian describing the junctions coupling $\mathcal{S}$ to the reservoirs. As time t goes to infinity, the coupled system approaches a steady state which carries a non-trivial entropy flux. The celebrated Landauer-Büttiker formula gives a closed expression for this steady state entropy flux in terms of the scattering data of the pair (h, h_0). This formula was rigorously proven in the context of non-equilibrium quantum statistical mechanics relatively recently [AJPP1, N][1]. Given the Landauer-Büttiker formula, the next natural question is the dependence of the steady state entropy flux on the structure of the sample $\mathcal{S}$ (its geometry, its size, *etc*). This paper is the first step in this direction of research.

We consider the special case where $\mathcal{S}$ is a finite one-dimensional structure described in the tight binding approximation by the single particle Hamiltonian $h_{\mathcal{S},L} = -\Delta_L + v$ on the Hilbert space $\ell^2([0, L] \cap \mathbb{Z})$. There Δ_L is the discrete Laplacian with Dirichlet boundary conditions and $v : \mathbb{Z}_+ \to \mathbb{R}$ is a potential on the half line $\mathbb{Z}_+ = \{0, 1, \cdots\}$. This finite sample is coupled to two infinitely extended reservoirs, one at each of its boundary point. The resulting steady state entropy flux may vanish in the limit $L \to \infty$ and our goal is to characterize the persistence of transport in this limit in terms of the spectral data of the limiting half-line Schrödinger operator $h_{\mathcal{S}} = -\Delta + v$ acting on $\ell^2(\mathbb{Z}_+)$.

We start with a precise description of the model and the problem we study.

1.1 Setup

The electronic black box (EBB) model we consider in this paper is a special case of the class of models studied in [AJPP1], where the reader can find the proofs of the results described in this introductory section. A pedagogical introduction to the topic can be found in the lecture notes [AJJP2].

Consider two free Fermi gases $\mathcal{R}_l$ and $\mathcal{R}_r$, colloquially called left and right reservoir, with single particle Hilbert space $\mathfrak{h}_l$ and $\mathfrak{h}_r$ and Hamiltonian h_l and h_r. The single particle Hilbert space $\mathfrak{h}_{\mathcal{S}}$ of the sample $\mathcal{S}$ is finite dimensional and its single particle Hamiltonian is $h_{\mathcal{S}}$. Until the very end of this section we shall not need to further specify the structure of $\mathcal{S}$. The EBB model we shall study is a free Fermi gas with single particle Hilbert space

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

The identity operators on $\mathfrak{h}$, $\mathfrak{h}_l$, $\mathfrak{h}_r$, $\mathfrak{h}_{\mathcal{S}}$ will be denoted 1, 1_l, 1_r, $1_{\mathcal{S}}$. Whenever the meaning is clear within the context, vectors and operators of the form $\psi \oplus 0$, $A \oplus 0$, $\ldots$ will be simply denoted by ψ, $A, \ldots$ Accordingly, 1_l, 1_r, $1_{\mathcal{S}}$ will be identified with the corresponding orthogonal projections in $\mathfrak{h}$.

For $f \in \mathfrak{h}$, we denote by $a(f)/a^*(f)$ the annihilation/creation operators on the antisymmetric (fermionic) Fock space $\mathcal{H} = \Gamma_-(\mathfrak{h})$ over $\mathfrak{h}$. In the sequel, $a^\#(f)$ stands for $a(f)$ or $a^*(f)$. The Hamiltonian of the decoupled EBB system is $H_0 = \mathrm{d}\Gamma(h_0)$, the second quantization of

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

The Hamiltonians and the number operators of the reservoirs are $H_{l/r} = \mathrm{d}\Gamma(h_{l/r})$ and $N_{l/r} = \mathrm{d}\Gamma(1_{l/r})$.

The algebra $\mathrm{CAR}(\mathfrak{h})$ of canonical anticommutation relations over $\mathfrak{h}$ is the C^*-algebra generated by the set of operators $\{a^\#(f) \,|\, f \in \mathfrak{h}\}$. To any self-adjoint operator k on $\mathfrak{h}$ one associates the Bogoliubov

[1] We refer the reader to these papers for additional information on the Landauer-Büttiker formula and for references to the vast physics literature on the subject.

group

$$\mathrm{b}_k^t(A) = \mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma(k)} A \mathrm{e}^{-\mathrm{i}t\mathrm{d}\Gamma(k)},$$

of automorphisms of $\mathrm{CAR}(\mathfrak{h})$. Note that

$$\mathrm{b}_k^t(a^\#(f)) = \mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma(k)} a^\#(f) \mathrm{e}^{-\mathrm{i}t\mathrm{d}\Gamma(k)} = a^\#(\mathrm{e}^{\mathrm{i}tk} f).$$

$\vartheta^t = \mathrm{b}_1^t$ is the gauge group of the EBB model. We shall assume that the total charge $N = \mathrm{d}\Gamma(1)$ is conserved. The corresponding superselection rule distinguishes the gauge-invariant sub-algebra

$$\mathrm{CAR}_\vartheta(\mathfrak{h}) = \{A \in \mathrm{CAR}(\mathfrak{h}) \,|\, \vartheta^t(A) = A \text{ for all } t\},$$

as the algebra of observables of the EBB model. The Bogoliubov group $\tau_0^t = \mathrm{b}_{h_0}^t$ preserves $\mathrm{CAR}_\vartheta(\mathfrak{h})$ and describes the time evolution of the decoupled EBB model. The pair $(\mathrm{CAR}_\vartheta(\mathfrak{h}), \tau_0^t)$ is a C^*-dynamical system.

For any self-adjoint operator ϱ on $\mathfrak{h}$ satisfying $0 \le \varrho \le 1$ the formula

$$\omega_\varrho(a^*(f_n)\cdots a^*(f_1)a(g_1)\cdots a(g_n)) = \det\{\langle g_i, \varrho f_j\rangle\},$$

defines a unique state ω_ϱ on $\mathrm{CAR}_\vartheta(\mathfrak{h})$. It is called the quasi-free state of density ϱ and is completely determined by its two point function

$$\omega_\varrho(a^*(f)a(g)) = \langle g, \varrho f\rangle.$$

The initial state of the EBB model is the quasi-free state ω_0 of density

$$\varrho_l \oplus \varrho_{\mathcal{S}} \oplus \varrho_r,$$

where $\varrho_{l/r}$ denotes the Fermi-Dirac density at inverse temperature $\beta_{l/r} > 0$ and chemical potential $\mu_{l/r} \in \mathbb{R}$,

$$\varrho_{l/r} = \frac{1_{l/r}}{1_{l/r} + \mathrm{e}^{\beta_{l/r}(h_{l/r} - \mu_{l/r} 1_{l/r})}}, \tag{1.1}$$

and $\varrho_{\mathcal{S}} = 1_{\mathcal{S}}$ (none of our results depends on this particular choice of $\varrho_{\mathcal{S}}$). ω_0 describes the thermodynamic state in which the reservoirs $\mathcal{R}_{l/r}$ are in thermal equilibrium at inverse temperatures $\beta_{l/r}$ and chemical potentials $\mu_{l/r}$.

The coupling we will consider is specified by a choice of non-zero vectors $\chi_{l/r} \in \mathfrak{h}_{l/r}$, $\psi_{l/r} \in \mathfrak{h}_{\mathcal{S}}$. The left/right junction is described by the rank two operator

$$h_{T,l/r} = |\chi_{l/r}\rangle\langle\psi_{l/r}| + |\psi_{l/r}\rangle\langle\chi_{l/r}|.$$

The single particle Hamiltonian of the coupled EBB model is

$$h = h_0 + h_T = h_0 + h_{T,l} + h_{T,r},$$

and its Hamiltonian is

$$H = \mathrm{d}\Gamma(h) = H_0 + a^*(\psi_l)a(\chi_l) + a^*(\chi_l)a(\psi_l) + a^*(\psi_r)a(\chi_r) + a^*(\chi_r)a(\psi_r).$$

The dynamics of the coupled EBB model is described by the Bogoliubov group $\tau^t = \mathrm{b}_h^t$. It preserves $\mathrm{CAR}_\vartheta(\mathfrak{h})$ and the pair $(\mathrm{CAR}_\vartheta(\mathfrak{h}), \tau^t)$ is a C^*-dynamical system. The coupled EBB model is described by the quantum dynamical system $(\mathrm{CAR}_\vartheta(\mathfrak{h}), \tau^t, \omega_0)$.

We now describe the energy/charge/entropy flux observables. Although the self-adjoint operators $H_{l/r}$ and $N_{l/r}$ are not in $\mathrm{CAR}(\mathfrak{h})$, the differences

$$\Delta H_{l/r}(t) = \mathrm{e}^{\mathrm{i}tH} H_{l/r} \mathrm{e}^{-\mathrm{i}tH} - H_{l/r}, \qquad \Delta N_{l/r}(t) = \mathrm{e}^{\mathrm{i}tH} N_{l/r} \mathrm{e}^{-\mathrm{i}tH} - N_{l/r},$$

belong to $\mathrm{CAR}_\vartheta(\mathfrak{h})$ for any $t \in \mathbb{R}$, and one easily verifies the relations

$$\Delta H_{l/r}(t) = -\int_0^t \tau^s(\Phi_{l/r})\mathrm{d}s, \qquad \Delta N_{l/r}(t) = -\int_0^t \tau^s(\mathcal{J}_{l/r})\mathrm{d}s,$$

where

$$\begin{aligned} \Phi_{l/r} &= -\mathrm{i}[H, H_{l/r}] = \mathrm{d}\Gamma(-\mathrm{i}[h, h_{l/r}]) = a^*(\mathrm{i}h_{l/r}\chi_{l/r})a(\psi_{l/r}) + a^*(\psi_{l/r})a(\mathrm{i}h_{l/r}\chi_{l/r}), \\ \mathcal{J}_{l/r} &= -\mathrm{i}[H, N_{l/r}] = \mathrm{d}\Gamma(-\mathrm{i}[h, 1_{l/r}]) = a^*(\mathrm{i}\chi_{l/r})a(\psi_{l/r}) + a^*(\psi_{l/r})a(\mathrm{i}\chi_{l/r}). \end{aligned} \tag{1.2}$$

The self-adjoint operators $\Phi_{l/r}$, $\mathcal{J}_{l/r}$ belong to $\mathrm{CAR}_\vartheta(\mathfrak{h})$ and are observables describing, respectively, the energy and charge flux out of the reservoir $\mathcal{R}_{l/r}$. The associated entropy flux observable is

$$\sigma = -\beta_l(\Phi_l - \mu_l \mathcal{J}_l) - \beta_r(\Phi_r - \mu_r \mathcal{J}_r). \tag{1.3}$$

We recall the entropy balance equation [JP, Ru]

$$\mathrm{Ent}(\omega_0 \circ \tau^t | \omega_0) = -\int_0^t \omega_0(\tau^s(\sigma))\mathrm{d}s, \tag{1.4}$$

where $\mathrm{Ent}(\,\cdot\,|\,\cdot\,)$ denotes Araki's relative entropy of two states [Ar][2]. Since $\mathrm{Ent}(\,\cdot\,|\,\cdot\,) \le 0$, the balance equation ensures that for all $t > 0$ the average entropy flux is non-negative,

$$\frac{1}{t}\int_0^t \omega_0(\tau^s(\sigma))\mathrm{d}s \ge 0, \tag{1.5}$$

in accordance with the second law of thermodynamics.

A basic characteristic of out of equilibrium physical systems is the presence of non-vanishing steady energy, charge and entropy fluxes. Sharp mathematical results concerning the existence and values of such fluxes can only be obtained in the idealization of the large time limit $t \to \infty$. To state the relevant result for the EBB model we need the assumption:

(H) The single particle Hamiltonian h has no singular continuous spectrum.

[2] The entropy balance equation holds in a much wider context and is a very general structural property of non-equilibrium statistical mechanics.

Theorem 1.1 ([AJPP1]) *Suppose that* (H) *holds. Then for all* $A \in \mathrm{CAR}_\vartheta(\mathfrak{h})$ *the limit*

$$\omega_+(A) = \lim_{t\to\infty} \frac{1}{t}\int_0^t \omega_0(\tau^s(A))\mathrm{d}s,$$

exists.

The functional ω_+ is a state on $\mathrm{CAR}_\vartheta(\mathfrak{h})$ and is called Non-Equilibrium Steady State (NESS) of the EBB model. The entropy balance equation (1.5) ensures that $\omega_+(\sigma) \geq 0$. The existence of ω_+ is an open problem if h has some singular continuous spectrum.

Although the existence of a NESS for a given quantum dynamical system is generally a difficult analytical problem, the special quasi-free structure of the EBB model reduces the proof of Theorem 1.1 to the study of the spectral and scattering theory of the pair (h, h_0). Moreover, the steady state expectation values $\omega_+(\Phi_{l/r})$, $\omega_+(\mathcal{J}_{l/r})$, $\omega_+(\sigma)$, can be expressed in closed form in terms of the scattering data of the pair (h, h_0). The resulting expressions, the celebrated Landauer-Büttiker formulae, were rigorously proven in [AJPP1, N] and yield natural necessary and sufficient conditions for the strict positivity of $\omega_+(\sigma)$. We proceed to describe the Landauer-Büttiker formulae and the question we will study in this paper.

We start with some basic observations about the EBB model. Let $\tilde{\mathfrak{h}}_{l/r} \subset \mathfrak{h}_{l/r}$ be the cyclic subspace generated by $h_{l/r}$ and $\chi_{l/r}$ (*i.e.*, the smallest $h_{l/r}$-invariant subspace of $\mathfrak{h}_{l/r}$ containing $\chi_{l/r}$). The Hilbert space

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

is invariant under h and h_0, and $\Phi_{l/r}, \mathcal{J}_{l/r}, \sigma \in \mathrm{CAR}_\vartheta(\tilde{\mathfrak{h}})$. Hence, for our purposes, w.l.o.g. we may replace $\mathfrak{h}_{l/r}$ and $\mathfrak{h}$ with $\tilde{\mathfrak{h}}_{l/r}$ and $\tilde{\mathfrak{h}}$ (we drop $\tilde{\cdot}$ in the sequel). Let $\nu_{l/r}$ be the spectral measure for $h_{l/r}$ and $\chi_{l/r}$. By the spectral theorem we may assume that $\mathfrak{h}_{l/r} = L^2(\mathbb{R}, \mathrm{d}\nu_{l/r})$, $\chi_{l/r}(E) = 1$ for all $E \in \mathbb{R}$, and that $h_{l/r}$ is the operator of multiplication by the variable E. It follows that the density operator (1.1) acts by multiplication with the function

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

The absolutely continuous spectral subspace of h_0 is

$$\mathfrak{h}_{\mathrm{ac}}(h_0) = \mathfrak{h}_{\mathrm{ac}}(h_l) \oplus \mathfrak{h}_{\mathrm{ac}}(h_r) = L^2(\mathbb{R}, \mathrm{d}\nu_{l,\mathrm{ac}}) \oplus L^2(\mathbb{R}, \mathrm{d}\nu_{r,\mathrm{ac}}),$$

where $\nu_{l/r,\mathrm{ac}}$ is the absolutely continuous part of $\nu_{l/r}$ (w.r.t. Lebesgue measure). To avoid discussion of trivialities we shall always assume that $\nu_{l/r,\mathrm{ac}}$ is non-zero (if either h_l or h_r has no absolutely continuous spectrum then $\omega_+(\Phi_{l/r}) = \omega_+(\mathcal{J}_{l/r}) = \omega_+(\sigma) = 0$, see [AJPP1]). The essential support of the measure $\nu_{l/r,\mathrm{ac}}$, defined by,

$$\Sigma_{l/r} = \left\{ E \in \mathbb{R} \,\middle|\, \frac{\mathrm{d}\nu_{l/r,\mathrm{ac}}}{\mathrm{d}E}(E) > 0 \right\},$$

is also called the essential support of the absolutely continuous spectrum of $h_{l/r}$. The intersection of the supports

$$\Sigma_{l\cap r} = \Sigma_l \cap \Sigma_r,$$

will play an important role in the sequel. As usual in measure theory, $\Sigma_{l/r}$ is only specified up to a set of Lebesgue measure zero. More precisely, it is an equivalence class of the relation

$$B_1 \mathrel{\hat{=}} B_2 \Leftrightarrow |B_1 \triangle B_2| = 0,$$

where B_1, B_2 are Borel sets and $|B|$ is the Lebesgue measure of B. As usual in measure theory we shall refer to such classes as sets.

Denote by $1_{\rm ac}(h_0)$ the orthogonal projection on $\mathfrak{h}_{\rm ac}(h_0)$. It follows from the trace class scattering theory that the wave operators

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

exist. The scattering matrix $s = w_+^* w_-$ is a unitary on $\mathfrak{h}_{\rm ac}(h_0)$ and acts as the operator of multiplication by a unitary 2×2 matrix function $s(E)$. We shall write this on-shell scattering matrix as

$$s(E) = 1 + t(E)$$

where

$$t(E) = \begin{bmatrix} t_{ll}(E) & t_{lr}(E) \\ t_{rl}(E) & t_{rr}(E) \end{bmatrix},$$

is the so-called t-matrix. The entry $t_{lr/rl}(E)$ is the transmission amplitude from reservoir $\mathcal{R}_{l/r}$ to the reservoir $\mathcal{R}_{r/l}$ at energy E and $|t_{lr/rl}(E)|^2$ is the corresponding transmission probability. We recall that, as a consequence of unitarity, $|t_{lr}(E)|^2 = |t_{rl}(E)|^2$. We set $\mathcal{T}(E) = |t_{lr}(E)|^2$ and notice that, as a consequence of formula (2.15)

$$\{E \,|\, \mathcal{T}(E) > 0\} \mathrel{\hat{=}} \Sigma_{l\cap r}. \tag{1.6}$$

Theorem 1.2 ([AJPP1]) *Suppose that* (H) *holds. The steady state energy and charge currents are given by the following Landauer-Büttiker formulae*

$$\omega_+(\Phi_{l/r}) = \frac{1}{2\pi}\int_{\mathbb{R}} \varphi_{l/r}(E){\rm d}E, \qquad \omega_+(\mathcal{J}_{l/r}) = \frac{1}{2\pi}\int_{\mathbb{R}} j_{l/r}(E){\rm d}E, \tag{1.7}$$

where

$$\varphi_{l/r}(E) = \mathcal{T}(E)(\varrho_{l/r}(E) - \varrho_{r/l}(E))E, \qquad j_{l/r}(E) = \mathcal{T}(E)(\varrho_{l/r}(E) - \varrho_{r/l}(E)). \tag{1.8}$$

Thus, one can identify the functions $\varphi_{l/r}$ and $j_{l/r}$ as the spectral densities of energy and charge current in the NESS ω_+. They satisfy the conservation laws

$$\varphi_l(E) + \varphi_r(E) = 0, \qquad j_l(E) + j_r(E) = 0.$$

By Eq. (1.3), the steady state entropy flux is given by

$$\omega_+(\sigma) = \frac{1}{2\pi}\int_{\mathbb{R}} \varsigma(E){\rm d}E, \tag{1.9}$$

where the spectral density

$$\begin{aligned}\varsigma(E) &= -\beta_l(\varphi_l(E) - \mu_l j_l(E)) - \beta_r(\varphi_r(E) - \mu_r j_r(E)) \\ &= \mathcal{T}(E)(\xi_r(E) - \xi_l(E))(\varrho_l(E) - \varrho_r(E)),\end{aligned} \tag{1.10}$$

is non-negative, and

$$\{E \,|\, \varsigma(E) > 0\} \doteq \{E \,|\, |\varphi_{l/r}(E)| > 0\} \doteq \{E \,|\, |j_{l/r}(E)| > 0\}.$$

If $\beta_l = \beta_r$ and $\mu_l = \mu_r$ (*the equilibrium case*), then $\varphi_{l/r}$, $j_{l/r}$, and ς are zero functions. If either $\beta_l \neq \beta_r$ or $\mu_l \neq \mu_r$ (*the non-equilibrium case*), then (1.6) implies

$$\{E \,|\, \varsigma(E) > 0\} \doteq \Sigma_{l\cap r}.$$

The functions $\varphi_{l/r}$, $j_{l/r}$ and ς are well defined and all the above properties hold even if h has some singular continuous spectrum. However, the current state of the art results require Assumption (H) to link these functions to steady state currents and prove the Landauer-Büttiker formulae (1.7).

Note that in the non-equilibrium case $\omega_+(\sigma) > 0$ iff $|\Sigma_{l\cap r}| > 0$, *i.e.*, $\omega_+(\sigma) > 0$ iff there exists an open scattering channel between $\mathcal{R}_l$ and $\mathcal{R}_r$. Note also that even if $\omega_+(\sigma) > 0$, it may happen that for some specific values of $\beta_{l/r}$, $\mu_{l/r}$ either $\omega_+(\Phi_{l/r}) = 0$ or $\omega_+(\mathcal{J}_{l/r}) = 0$. However, in the non-equilibrium case, $\omega_+(\Phi_{l/r})$ and $\omega_+(\mathcal{J}_{l/r})$ cannot simultaneously vanish and generically they are both different from zero.

We now describe the question we shall study. Let $v : \mathbb{Z}_+ \to \mathbb{R}$ be a given potential. Consider the finite lattice $\Gamma_L = [0, L] \cap \mathbb{Z}_+$ and suppose that the single particle Hilbert space and Hamiltonian of the sample are $\mathfrak{h}_{\mathcal{S},L} = \ell^2(\Gamma_L)$ and $h_{\mathcal{S},L} = -\Delta_L + v_L$, where $(\Delta_L u)(x) = u(x-1) + u(x+1)$ is the discrete Laplacian on Γ_L with Dirichlet boundary conditions (*i.e.*, $u(-1) = u(L+1) = 0$) and v_L is the restriction of the potential v to Γ_L. The reservoirs $\mathcal{R}_{l/r}$ and the vector $\chi_{l/r}$ are L independent. We take $\psi_l = \delta_0$, $\psi_r = \delta_L$ where δ_x denotes the usual Kronecker delta at $x \in \Gamma_L$. We denote by $h_{T,L}$ the corresponding tunneling Hamiltonian and set

$$h_L = h_{0,L} + h_{T,L}, \qquad h_{0,L} = h_l \oplus h_{\mathcal{S},L} \oplus h_r.$$

Denote by $\varphi_{l/r,L}$, $j_{l/r,L}$ and ς_L the spectral densities of the steady state fluxes and let

$$\begin{aligned}\overline{\mathfrak{T}} &= \{E \,|\, \limsup_{L\to\infty} \varsigma_L(E) > 0\}, \\ \underline{\mathfrak{T}} &= \{E \,|\, \liminf_{L\to\infty} \varsigma_L(E) > 0\}.\end{aligned} \tag{1.11}$$

Clearly, $\underline{\mathfrak{T}} \subset \overline{\mathfrak{T}} \subset \Sigma_{l\cap r}$. Note also that

$$\overline{\mathfrak{T}} = \{E \,|\, \limsup_{L\to\infty} |\varphi_{l/r,L}(E)| > 0\} = \{E \,|\, \limsup_{L\to\infty} |j_{l/r,L}(E)| > 0\},$$

and similarly for $\underline{\mathfrak{T}}$.

Let $h_{\mathcal{S}} = -\Delta + v$ be the limiting half-line Schrödinger operator acting on $\ell^2(\mathbb{Z}_+)$. If $h_{\mathcal{S},L}$ is extended from $\ell^2(\Gamma_L)$ to $\ell^2(\mathbb{Z}_+)$ in the obvious way (by setting $h_{\mathcal{S},L} = 0$ on $\ell^2(\Gamma_L)^\perp$), then $\lim_{L\to\infty} h_{\mathcal{S},L} = h_{\mathcal{S}}$

in the strong resolvent sense. δ_0 is a cyclic vector for $h_{\mathcal{S}}$ and the corresponding spectral measure $\nu_{\mathcal{S}}$ contains the full spectral information about $h_{\mathcal{S}}$. The set

$$\Sigma_{\mathcal{S}} = \left\{ E \,\middle|\, \frac{\mathrm{d}\nu_{\mathcal{S},\mathrm{ac}}}{\mathrm{d}E}(E) > 0 \right\},$$

is the essential support of the absolutely continuous spectrum of $h_{\mathcal{S}}$. On physical grounds, it is natural to introduce:

> **Property RST.** The half-line Schrödinger operator $h_{\mathcal{S}}$ exhibits regular spectral transport if for any choice of the reservoirs $\mathcal{R}_{l/r}$,
>
> $$\underline{\mathfrak{T}} \doteq \overline{\mathfrak{T}} \doteq \Sigma_{\mathcal{S}} \cap \Sigma_{l\cap r}. \tag{1.12}$$

In the first version of this paper we have conjectured that Property RST holds for all potentials v and we will comment further on this point in the next section. If Property RST holds and the reservoirs are chosen so that $\Sigma_{\mathcal{S}} \subset \Sigma_{l\cap r}$, then $\Sigma_{\mathcal{S}}$ is precisely the set of energies at which transport persists in the limit $L \to \infty$. Moreover, by Fatou's lemma, for any Borel set $B \subset \Sigma_{\mathcal{S}}$ of positive Lebesgue measure,

$$\liminf_{L\to\infty} \int_B \varsigma_L(E)\mathrm{d}E > 0,$$

while the dominated convergence theorem implies

$$\lim_{L\to\infty} \int_{\mathbb{R}\setminus\Sigma_{\mathcal{S}}} \varsigma_L(E)\mathrm{d}E = 0.$$

Hence the essential support of the absolutely continuous spectrum of operators satisfying (1.12) has a physically natural characterization in terms of transport.

Our main result gives sharp characterizations of the sets $\overline{\mathfrak{T}}$ and $\underline{\mathfrak{T}}$ in terms of the growth of the norms of the transfer matrices associated to $h_{\mathcal{S}}$. This characterization shows that Property RST holds for the potential v if and only if the celebrated Schrödinger conjecture (Property SC in the next section) holds for v. This equivalence, which came as a surprise to us, links properties of generalized eigenfunctions with the mechanism of non-equilibrium transport in this class of EBB models.

1.2 Results

Since in the equilibrium case ς_L is identically equal to zero, in what follows we assume the non-equilibrium case, *i.e.*, that either $\beta_l \neq \beta_r$ or $\mu_l \neq \mu_r$.

The transfer matrix at energy E is defined by the product

$$T_L(E) = \begin{bmatrix} v(L) - E & -1 \\ 1 & 0 \end{bmatrix} \cdots \begin{bmatrix} v(0) - E & -1 \\ 1 & 0 \end{bmatrix}. \tag{1.13}$$

We denote by $\mathfrak{L}$ the collection of all sequences $(L_k)_{k\in\mathbb{N}}$ of positive integers such that $L_k \uparrow \infty$. Our main results is

Theorem 1.3 *There is a set S in the equivalence class of $\Sigma_{l\cap r}$ such that, for any $E \in S$ and any $(L_k)_{k\in\mathbb{N}} \in \mathfrak{L}$, the following statements are equivalent.*

(1)
$$\lim_{k\to\infty} \varsigma_{L_k}(E) = 0.$$

(2)
$$\lim_{k\to\infty} \|T_{L_k}(E)\| = \infty.$$

Let
$$\mathfrak{S}_0 = \left\{ E \,\middle|\, \sup_L \|T_L(E)\| < \infty \right\}, \qquad \mathfrak{S}_1 = \left\{ E \,\middle|\, \liminf_{L\to\infty} \|T_L(E)\| < \infty \right\}.$$

An immediate consequence of Theorem 1.3 is

Corollary 1.4 (1)
$$\underline{\mathfrak{T}} \doteq \mathfrak{S}_0 \cap \Sigma_{l\cap r}.$$

(2)
$$\overline{\mathfrak{T}} \doteq \mathfrak{S}_1 \cap \Sigma_{l\cap r}.$$

(3) *For any Borel set $B \subset \mathfrak{S}_0 \cap \Sigma_{l\cap r}$ of positive Lebesgue measure,*
$$\liminf_{L\to\infty} \int_B \varsigma_L(E)\mathrm{d}E > 0.$$

(4)
$$\lim_{L\to\infty} \int_{\mathbb{R}\setminus(\mathfrak{S}_1\cap\Sigma_{l\cap r})} \varsigma_L(E)\mathrm{d}E = 0.$$

It follows from Corollary 1.4 that Property RST is equivalent to

Property SC. $\mathfrak{S}_0 \doteq \Sigma_{\mathcal{S}} \doteq \mathfrak{S}_1$.

Until recently, it was widely believed that Property SC holds for all potentials v (see [MMG] and Section C5 in [S1]), a fact known as Schrödinger Conjecture. Regarding the existing results, the inclusion $\mathfrak{S}_0 \subset \Sigma_{\mathcal{S}}$ was proven in [GP, KP] (see also [S2]). The inclusion $\Sigma_{\mathcal{S}} \subset \mathfrak{S}_1$ was proven in [LS]. After this work was completed and submitted for publication we have learned that Arthur Avila has announced a counterexample to the Schrödinger conjecture in the setting of ergodic Schrödinger operators [Av].

Property SC plays a central role in the spectral theory of one-dimensional Schrödinger operators. Theorem 1.3 and Corollary 1.4 link this property, via the Landauer-Büttiker formula, to non-equilibrium transport and shed a new light on its physical interpretation.[3] Property SC appears very natural from

[3] We remark that to link Corollary 1.4 with transport in non-equilibrium statistical mechanics one needs that the Landauer-Büttiker formulae hold for all L and hence that the coupled single particle Hamiltonian h_L has no singular continuous spectrum for all L. A concrete example of reservoirs where this is the case for any potential v 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].

the point of view of transport theory and its failure provides examples of models with strikingly singular non-equilibrium transport. In particular, the transport properties of Avila's spectacular counterexample remain to be studied in the future.

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2 Proofs

2.1 Preliminaries

We will denote by $\mathrm{sp}(A)$ the spectrum of a Hilbert space operator A, and write $\mathrm{Im}\, A = (A - A^*)/2\mathrm{i}$. If A is self-adjoint, then $\mathrm{sp}_{\mathrm{ac}}(A)$ denotes its absolutely continuous spectrum and we write $A > 0$ whenever $\mathrm{sp}(A) \subset]0, \infty[$.

In the following, we shall use indices $a, b, c, \ldots \in \{l, r\}$. We define

$$F_a(z) = \langle \chi_a, (h_a - z)^{-1} \chi_a \rangle,$$

and denote by $F(z)$ the 2×2 diagonal matrix with entries $F_{ab}(z) = \delta_{ab} F_a(z)$. We also introduce the 2×2 Green matrices $G_L^{(0)}(z)$ and $G_L(z)$ with entries

$$G_{ab,L}^{(0)}(z) = \langle \psi_a, (h_{\mathcal{S},L} - z)^{-1} \psi_b \rangle, \qquad G_{ab,L}(z) = \langle \psi_a, (h_L - z)^{-1} \psi_b \rangle.$$

Next, we recall several basic facts regarding the boundary values of the resolvent and their role in spectral theory. A pedagogical introduction to this topic, including complete proofs, can be found in [J]. Let A be a self-adjoint operator on a Hilbert space $\mathfrak{H}$ and $\psi_1, \psi_2 \in \mathfrak{H}$. For Lebesgue a.e. $E \in \mathbb{R}$ the boundary values

$$\langle \psi_1, (A - E - \mathrm{i}0)^{-1} \psi_2 \rangle = \lim_{\epsilon \downarrow 0} \langle \psi_1, (A - E - \mathrm{i}\epsilon)^{-1} \psi_2 \rangle, \tag{2.14}$$

exist and are finite. In the sequel, whenever we write $\langle \psi_1, (A - E - \mathrm{i}0)^{-1} \psi_2 \rangle$, we will always assume that the limit exists and is finite. If the spectral measure ν_{ψ_1,ψ_2} for A and ψ_1, ψ_2 is real-valued, then either ψ_1 is orthogonal to the cyclic subspace spanned by A and ψ_2 and ν_{ψ_1,ψ_2} is the zero measure or $\langle \psi_1, (A - E - \mathrm{i}0)^{-1} \psi_2 \rangle \neq 0$ for Lebesgue a.e. $E \in \mathbb{R}$. If $\psi \in \mathfrak{H}$ then $\mathrm{Im}\, \langle \psi, (A - E - \mathrm{i}0)^{-1} \psi \rangle \geq 0$ and if ν_ψ is the spectral measure for A and ψ, then

$$\mathrm{d}\nu_{\psi,\mathrm{ac}}(E) = \frac{1}{\pi} \mathrm{Im}\, \langle \psi, (A - E - \mathrm{i}0)^{-1} \psi \rangle \mathrm{d}E,$$

so that the set $\{E \,|\, \mathrm{Im}\, \langle \psi, (A - E - \mathrm{i}0)^{-1} \psi \rangle > 0\}$ is an essential support of $\nu_{\psi,\mathrm{ac}}$.

In particular, one has

$$\mathrm{d}\nu_{l/r,\mathrm{ac}}(E) = \frac{1}{\pi}\mathrm{Im}\, F_{l/r}(E+\mathrm{i}0)\mathrm{d}E,$$

and, with a slight abuse of notation, we may denote the following concrete representative of the class $\Sigma_{l\cap r}$ by the same letter

$$\{E \,|\, \mathrm{Im}\, F(E+\mathrm{i}0) > 0\} = \Sigma_{l\cap r}.$$

In words, $\Sigma_{l\cap r}$ consists of E's for which the boundary values $F_{l/r}(E+\mathrm{i}0)$ exist, are finite, and have strictly positive imaginary part.

2.2 Green's and transfer matrices

It follows from stationary scattering theory (see [Y], Chap. 5) that the t-matrix t_L can be expressed in terms of the Green matrix G_L by

$$t_L(E) = 2\mathrm{i}(\mathrm{Im}\, F(E+\mathrm{i}0))^{1/2} G_L(E+\mathrm{i}0)(\mathrm{Im}\, F(E+\mathrm{i}0))^{1/2}. \tag{2.15}$$

The formulae (2.15) can be also proven directly by elementary means following the arguments in [JKP]. The unitarity of the on shell scattering matrix $s_L(E) = 1 + t_L(E)$ implies that for Lebesgue a.e. $E \in \mathbb{R}$,

$$t_L^*(E)t_L(E) + t_L(E) + t_L^*(E) = 0. \tag{2.16}$$

It follows that

$$\mathfrak{R} = \bigcap_L \{E \in \Sigma_{l\cap r} \,|\, \text{Eqs. (2.15) and (2.16) hold}\},$$

satisfies

$$\Sigma_{l\cap r} \mathrel{\hat{=}} \mathfrak{R}.$$

The following lemma relates the Green matrices $G_L^{(0)}$ and G_L.

Lemma 2.1 *For $E \in \mathfrak{R} \setminus \mathrm{sp}(h_{\mathcal{S},L})$, one has $G_L^{(0)}(E) = (I - G_L^{(0)}(E)F(E+\mathrm{i}0))G_L(E+\mathrm{i}0)$.*

Proof. For $z \in \mathbb{C} \setminus \mathbb{R}$, the second resolvent formula

$$(h_L - z)^{-1} - (h_{0,L} - z)^{-1} = -(h_{0,L} - z)^{-1} h_{T,L} (h_L - z)^{-1},$$

yields

$$G_{ab}(z) - G_{ab}^{(0)}(z) = -\sum_c G_{ac}^{(0)}(z)\langle \chi_c, (h_L - z)^{-1}\psi_b\rangle,$$

and

$$\langle \chi_c, (h_L - z)^{-1}\psi_b\rangle = -F_c(z)G_{cb}(z),$$

which combine to give the desired formula. □

We proceed to relate the Green matrix $G_L^{(0)}$ with the transfer matrix (1.13).

Lemma 2.2 *For $E \in \mathbb{R} \setminus \mathrm{sp}(h_{\mathcal{S},L})$ and any $x, y, u, v \in \mathbb{C}$ one has*

$$G_L^{(0)}(E) \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} u \\ v \end{bmatrix} \Longleftrightarrow T_L(E) \begin{bmatrix} u \\ x \end{bmatrix} = \begin{bmatrix} y \\ v \end{bmatrix}.$$

In other words, the permutation matrix $P^{(0)} : (x, y, u, v) \mapsto (u, x, y, v)$ maps the graph of $G_L^{(0)}(E)$ into that of $T_L(E)$.

Proof. Fix L and $E \in \mathbb{R} \setminus \mathrm{sp}(h_{\mathcal{S},L})$. For $f \in \ell^2(\Gamma_L)$, the function $\psi(x) = \langle \delta_x, (h_{\mathcal{S},L} - E)^{-1} f \rangle$ satisfies the finite difference equation

$$(-\Delta + v - E)\psi = f, \tag{2.17}$$

with boundary conditions $\psi(-1) = \psi(L+1) = 0$. Using the transfer matrix

$$T(x, y) = T_x T_{x-1} \cdots T_{y+1}, \qquad T_j = \begin{bmatrix} v(j) - E & -1 \\ 1 & 0 \end{bmatrix},$$

the solution of the initial value problem for Equ. (2.17) can be written as

$$\begin{bmatrix} \psi(x+1) \\ \psi(x) \end{bmatrix} = T(x, -1) \begin{bmatrix} \psi(0) \\ \psi(-1) \end{bmatrix} - \sum_{z=0}^{x} T(x, z) \begin{bmatrix} f(z) \\ 0 \end{bmatrix}.$$

Setting $x = L$ and taking the boundary conditions into account yields

$$T_L(E) \begin{bmatrix} \psi(0) \\ 0 \end{bmatrix} - \begin{bmatrix} 0 \\ \psi(L) \end{bmatrix} = \sum_{z=0}^{L} T(L, z) \begin{bmatrix} f(z) \\ 0 \end{bmatrix},$$

which is an equation for the unknown $\psi(0)$ and $\psi(L)$. Setting $f = \delta_0$ and $f = \delta_L$, we obtain the following equations for the entries of the matrix $G_L^{(0)}(E)$,

$$T_L(E) \begin{bmatrix} G_{ll,L}^{(0)}(E) \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ G_{rl,L}^{(0)}(E) \end{bmatrix}, \qquad T_L(E) \begin{bmatrix} G_{lr,L}^{(0)}(E) \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ G_{rr,L}^{(0)}(E) \end{bmatrix}.$$

Thus, the two linearly independent vectors $(G_{ll,L}^{(0)}(E), 1, 0, G_{rl,L}^{(0)}(E))$ and $(G_{lr,L}^{(0)}(E), 0, 1, G_{rr,L}^{(0)}(E))$ span the graph of $T_L(E)$. One easily checks that they are the images by the permutation matrix $P^{(0)}$ of the two vectors $(1, 0, G_{ll,L}^{(0)}(E), G_{rl,L}^{(0)}(E))$ and $(0, 1, G_{lr,L}^{(0)}(E), G_{rr,L}^{(0)}(E))$ which span the graph of $G_L^{(0)}(E)$. □

Combining the two previous lemmata, we obtain the connection between the transfer matrix and the Green matrix $G(E + \mathrm{i}0)$.

Lemma 2.3 *For $E \in \Re \setminus \mathrm{sp}(h_{\mathcal{S},L})$ and any $x, y, u, v \in \mathbb{C}$ one has*

$$G_L(E + \mathrm{i}0) \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} u \\ v \end{bmatrix} \Longleftrightarrow T_L(E) \begin{bmatrix} u \\ x + F_l(E + \mathrm{i}0)u \end{bmatrix} = \begin{bmatrix} y + F_r(E + \mathrm{i}0)v \\ v \end{bmatrix}.$$

In other words, the automorphism $P : (x, y, u, v) \mapsto (u, x + F_l(E + \mathrm{i}0)u, y + F_r(E + \mathrm{i}0)v, v)$ of $\mathbb{C}^4$ maps the graph of $G_L(E + \mathrm{i}0)$ into that of $T_L(E)$.

2.3 Proof of Theorem 1.3

Formulas (1.10) and (2.15) imply that Theorem 1.3 follows from

Theorem 2.4 *Let* $E \in \mathfrak{R} \setminus (\cup_L \mathrm{sp}(h_{\mathcal{S},L})) \mathrel{\hat{=}} \Sigma_{l\cap r}$ *and* $(L_k)_{k\in\mathbb{N}} \in \mathfrak{L}$ *be given. Then the following statements are equivalent.*

(1)

$$\lim_{k\to\infty} G_{lr,L_k}(E+\mathrm{i}0) = 0.$$

(2)

$$\lim_{k\to\infty} \|T_{L_k}(E)\| = \infty.$$

Proof. (1) $\Rightarrow$ (2). We start with the observation that the unitarity relation (2.16) implies $\|t_L(E)\| \leq 2$. It follows from (2.15) that the sequence $\|G_{L_k}(E+\mathrm{i}0)\|$ is bounded. Writing

$$G_{L_k}(E+\mathrm{i}0)\begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} u_k \\ v_k \end{bmatrix},$$

we conclude that the sequences u_k and v_k are bounded while (1) implies $u_k = G_{lr,L_k}(E+\mathrm{i}0) \to 0$. It follows from Lemma 2.3 that

$$T_{L_k}(E)\begin{bmatrix} 1 \\ F_l(E+\mathrm{i}0) \end{bmatrix} = \frac{1}{u_k}\begin{bmatrix} 1 + F_r(E+\mathrm{i}0)v_k \\ v_k \end{bmatrix},$$

which clearly implies (2).

(2) $\Rightarrow$ (1). There exists bounded sequences u_k and x_k such that, writing

$$T_{L_k}(E)\begin{bmatrix} u_k \\ x_k + F_l(E+\mathrm{i}0)u_k \end{bmatrix} = \begin{bmatrix} y_k + F_r(E+\mathrm{i}0)v_k \\ v_k \end{bmatrix},$$

the sequence $|v_k| + |y_k|$ diverges to infinity. By Lemma 2.3, one has

$$G_{L_k}(E+\mathrm{i}0)\begin{bmatrix} x_k \\ y_k \end{bmatrix} = \begin{bmatrix} u_k \\ v_k \end{bmatrix},$$

and the boundedness of $\|G_{L_k}(E+\mathrm{i}0)\|$ implies that $|v_k| \leq A + B|y_k|$ for some positive constants A and B. We conclude that $|y_k| \to \infty$ and (1) follows from

$$G_{lr,L_k}(E+\mathrm{i}0) = \frac{u_k - G_{ll,L_k}(E+\mathrm{i}0)x_k}{y_k}.$$

□

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