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 $S$ connected at its left and right ends to two infinitely extended reservoirs $R_l, r$ 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 $h_{S, L} = -\Delta + v$. The Landauer-Büttiker formula expresses the steady state entropy flux in the coupled system $R_l + S + R_r$ 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 $h_S$.

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 $S$ (e.g., a quantum dot or a more elaborate electronic device) coupled to several electronic reservoirs $R_j$. These reservoirs are free Fermi gas in thermal equilibrium at given temperatures and chemical potentials. In the independent electron approximation, the coupled system $S + \sum_j R_j$ is a free Fermi gas with single particle Hamiltonian $h = h_0 + h_T$, where $h_0$ is the single particle Hamiltonian of the decoupled system and $h_T$ is the tunneling Hamiltonian describing the junctions coupling $S$ 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 \([\text{AJPP1}, \text{N}]\). Given the Landauer-Büttiker formula, the next natural question is the dependence of the steady state entropy flux on the structure of the sample \(S\) (its geometry, its size, etc). This paper is the first step in this direction of research.

We consider the special case where \(S\) is a finite one-dimensional structure described in the tight binding approximation by the single particle Hamiltonian \(h_{S,L} = -\Delta_L + v\) on the Hilbert space \(\ell^2([0, L] \cap \mathbb{Z})\). There \(\Delta_L\) is the discrete Laplacian with Dirichlet boundary conditions and \(v : \mathbb{Z}_+ \rightarrow \mathbb{R}\) 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 points. The resulting steady state entropy flux may vanish in the limit \(L \rightarrow \infty\) 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 \(h_S = -\Delta + v\) 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 \([\text{AJPP1}]\), 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 \([\text{AJJP2}]\).

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

\[
h = h_l \oplus h_S \oplus h_r.\]

The identity operators on \(h\), \(h_l\), \(h_r\), \(h_S\) will be denoted \(1, 1_l, 1_r, 1_S\). 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 \(\psi, A, \ldots\) Accordingly, \(1_l, 1_r, 1_S\) will be identified with the corresponding orthogonal projections in \(h\).

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

\[
h_0 = h_l \oplus h_S \oplus h_r.\]

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

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

\[
h^\dagger_k(A) = e^{itd\Gamma(k)}Ae^{-itd\Gamma(k)},\]

\(\text{We refer the reader to these papers for additional information on the Landauer-Büttiker formula and for references to the vast physics literature on the subject.}\)
of automorphisms of CAR(\(\mathfrak{h}\)). Note that
\[
b_t^k(a^\#(f)) = e^{\imath t \Gamma(k)} a^\#(f) e^{-\imath t \Gamma(k)} = a^\#(e^{\imath t k} f).
\]
\(\vartheta^t = b_t^1\) is the gauge group of the EBB model. We shall assume that the total charge \(N = d \Gamma(1)\) is conserved. The corresponding superselection rule distinguishes the gauge-invariant sub-algebra
\[
\text{CAR}_{\vartheta}(\mathfrak{h}) = \{ A \in \text{CAR}(\mathfrak{h}) \mid \vartheta^t(A) = A \text{ for all } t \},
\]
as the algebra of observables of the EBB model. The Bogoliubov group \(\tau^t = b_t^1\) preserves \(\text{CAR}_{\vartheta}(\mathfrak{h})\) and describes the time evolution of the decoupled EBB model. The pair \((\text{CAR}_{\vartheta}(\mathfrak{h}), \tau^t)\) is a \(C^*\)-dynamical system.

For any self-adjoint operator \(\varrho\) on \(\mathfrak{h}\) satisfying \(0 \leq \varrho \leq 1\) 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 \(\omega_{\varrho}\) on \(\text{CAR}_{\vartheta}(\mathfrak{h})\). It is called the quasi-free state of density \(\varrho\) 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 \(\omega_0\) of density
\[
\varrho_l \oplus \varrho_S \oplus \varrho_r,
\]
where \(\varrho_{l/r}\) denotes the Fermi-Dirac density at inverse temperature \(\beta_{l/r} > 0\) and chemical potential \(\mu_{l/r} \in \mathbb{R}\),
\[
\varrho_{l/r} = \frac{1_{l/r}}{1_{l/r} + e^{\beta_{l/r} (h_{l/r} - \mu_{l/r} 1_{l/r})}}, \quad (1.1)
\]
and \(\varrho_S = 1_S\) (none of our results depends on this particular choice of \(\varrho_S\)). \(\omega_0\) describes the thermodynamic state in which the reservoirs \(R_{l/r}\) 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 \(\chi_{l/r} \in \mathfrak{h}_{l/r}, \psi_{l/r} \in \mathfrak{h}_S\). 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
\[
H = d \Gamma(h) = H_0 + a^*(\psi_l)a(\chi_l) + a^*(\chi_l)a(\psi_l) + a^*(\psi_r)a(\chi_r) + a^*(\chi_r)a(\psi_r).
\]
The dynamics of the coupled EBB model is described by the Bogoliubov group \(\tau^t = b_t^1\). It preserves \(\text{CAR}_{\vartheta}(\mathfrak{h})\) and the pair \((\text{CAR}_{\vartheta}(\mathfrak{h}), \tau^t)\) is a \(C^*\)-dynamical system. The coupled EBB model is described by the quantum dynamical system \((\text{CAR}_{\vartheta}(\mathfrak{h}), \tau^t, \omega_0)\).
We now describe the energy/charge/entropy flux observables. Although the self-adjoint operators $H_{l/r}$ and $N_{l/r}$ are not in $\text{CAR}(h)$, the differences
\[ \Delta H_{l/r}(t) = e^{itH} H_{l/r} e^{-itH} - H_{l/r}, \quad \Delta N_{l/r}(t) = e^{itH} N_{l/r} e^{-itH} - N_{l/r}, \]
belong to $\text{CAR}_0(h)$ for any $t \in \mathbb{R}$, and one easily verifies the relations
\[ \Delta H_{l/r}(t) = - \int_0^t \tau^s(\Phi_{l/r}) \, ds, \quad \Delta N_{l/r}(t) = - \int_0^t \tau^s(J_{l/r}) \, ds, \]
where
\[
\Phi_{l/r} = -i[H, H_{l/r}] = d\Gamma(-i[h, h_{l/r}]) = a^*(ih_{l/r}\chi_{l/r})a(\psi_{l/r}) + a^*(\psi_{l/r})a(ih_{l/r}\chi_{l/r}),
\]
\[
J_{l/r} = -i[H, N_{l/r}] = d\Gamma(-i[h, 1_{l/r}]) = a^*(i\chi_{l/r})a(\psi_{l/r}) + a^*(\psi_{l/r})a(i\chi_{l/r}).
\] (1.2)

The self-adjoint operators $\Phi_{l/r}, J_{l/r}$ belong to $\text{CAR}_0(h)$ and are observables describing, respectively, the energy and charge flux out of the reservoir $\mathcal{R}_{l/r}$. The associated entropy flux observable is
\[ \sigma = -\beta_l(\Phi_l - \mu_l J_l) - \beta_r(\Phi_r - \mu_r J_r). \] (1.3)

We recall the entropy balance equation [JP, Ru]
\[ \text{Ent}(\omega_0 \circ \tau^t|\omega_0) = - \int_0^t \omega_0(\tau^s(\sigma)) \, ds, \] (1.4)
where $\text{Ent}(\cdot|\cdot)$ denotes Araki’s relative entropy of two states [Ar].$^2$ Since $\text{Ent}(\cdot|\cdot) \leq 0$, the balance equation ensures that for all $t > 0$ the average entropy flux is non-negative,
\[ \frac{1}{t} \int_0^t \omega_0(\tau^s(\sigma)) \, ds \geq 0, \] (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.

**Theorem 1.1** ([AJPP1]) *Suppose that (H) holds. Then for all $A \in \text{CAR}_0(h)$ the limit
\[ \omega_+(A) = \lim_{t \to \infty} \frac{1}{t} \int_0^t \omega_0(\tau^s(A)) \, ds, \]
exists.*

$^2$The entropy balance equation holds in a much wider context and is a very general structural property of non-equilibrium statistical mechanics.
The functional $\omega_+$ is a state on $\text{CAR}_\rho(\mathfrak{h})$ 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 $\omega_+$ 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 $\tilde{h}_{l/r} \subset h_{l/r}$ be the cyclic subspace generated by $h_{l/r}$ and $\chi_{l/r}$ (i.e., the smallest $h_{l/r}$-invariant subspace of $h_{l/r}$ containing $\chi_{l/r}$). The Hilbert space

$$\tilde{\mathfrak{h}} = \tilde{h}_{l/r} \oplus \mathfrak{h}_S \oplus \tilde{h}_{r},$$

is invariant under $h$ and $h_0$, and $\Phi_{l/r}, J_{l/r}, \sigma \in \text{CAR}_\rho(\tilde{h})$. Hence, for our purposes, w.l.o.g. we may replace $h_{l/r}$ and $h$ with $\tilde{h}_{l/r}$ and $\tilde{h}$ (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 $h_{l/r} = \mathcal{L}^2(\mathbb{R}, d\nu_{l/r}), \chi_{l/r}(E) = 1$ 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

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

The absolutely continuous spectral subspace of $h_0$ is

$$\mathfrak{h}_{ac}(h_0) = \mathfrak{h}_{ac}(\tilde{h}_{l/r}) \oplus \mathfrak{h}_{ac}(\tilde{h}_{r}) = \mathcal{L}^2(\mathbb{R}, d\nu_{l/r,ac}) \oplus \mathcal{L}^2(\mathbb{R}, d\nu_{r,ac}),$$

where $\nu_{l/r,ac}$ is the absolutely continuous part of $\nu_{l/r}$ (w.r.t. Lebesgue measure). To avoid discussion of trivialities we shall always assume that $\nu_{l/r,ac}$ is non-zero (if either $\tilde{h}_{l/r}$ or $h_{l/r}$ 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 $\nu_{l/r,ac}$, defined by,

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

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

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

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

$$B_1 \equiv B_2 \Leftrightarrow |B_1 \Delta B_2| = 0,$$

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 \( 1_{\text{ac}}(h_0) \) the orthogonal projection on \( h_{\text{ac}}(h_0) \). It follows from the trace class scattering theory that the wave operators

\[
w_+ = s - \lim_{t \to \pm \infty} e^{ith_0} 1_{\text{ac}}(h_0),
\]

exist. The scattering matrix \( s = w_+^* w_- \) is a unitary on \( h_{\text{ac}}(h_0) \) and acts as the operator of multiplication by a unitary \( 2 \times 2 \) 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 \( t_{lr}(E) \) is the transmission amplitude from reservoir \( R_l \) to the reservoir \( R_r \) at energy \( E \) and \( |t_{lr}(E)|^2 \) 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)

\[
\{ E | \mathcal{T}(E) > 0 \} = \Sigma_{l\cap r}. \tag{1.6}
\]

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

\[
\omega_+(\Phi_{l/r}) = \frac{1}{2\pi} \int_{\mathbb{R}} \phi_{l/r}(E) dE, \quad \omega_+(\mathcal{J}_{l/r}) = \frac{1}{2\pi} \int_{\mathbb{R}} j_{l/r}(E) dE, \tag{1.7}
\]

where

\[
\phi_{l/r}(E) = \mathcal{T}(E)(\varrho_{l/r}(E) - \varrho_{r/l}(E))E, \quad j_{l/r}(E) = \mathcal{T}(E)(\varrho_{l/r}(E) - \varrho_{r/l}(E)). \tag{1.8}
\]

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

\[
\phi_l(E) + \phi_r(E) = 0, \quad j_l(E) + j_r(E) = 0.
\]

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

\[
\omega_+(\sigma) = \frac{1}{2\pi} \int_{\mathbb{R}} \varsigma(E) dE, \tag{1.9}
\]

where the spectral density

\[
\varsigma(E) = -\beta_l(\phi_l(E) - \mu_l j_l(E)) - \beta_r(\phi_r(E) - \mu_r j_r(E))
\]

\[
= T(E)(\xi_r(E) - \xi_l(E))(\varrho_l(E) - \varrho_r(E)), \tag{1.10}
\]

is non-negative, and

\[
\{ E | \varsigma(E) > 0 \} = \{ E | |\phi_{l/r}(E)| > 0 \} \overset{\text{def}}{=} \{ E | |j_{l/r}(E)| > 0 \}.
\]
If \( \beta_l = \beta_r \) and \( \mu_l = \mu_r \) \((\text{the equilibrium case})\), then \( \varphi_{l/r}, \mathcal{J}_{l/r}, \) and \( \varsigma \) are zero functions. If either \( \beta_l \neq \beta_r \) or \( \mu_l \neq \mu_r \) \((\text{the non-equilibrium case})\), then (1.6) implies
\[
\{ E \mid \varsigma(E) > 0 \} = \Sigma_{l/r}.
\]
The functions \( \varphi_{l/r}, \mathcal{J}_{l/r}, \) and \( \varsigma \) 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 \( |\Sigma_{l/r}| > 0 \), 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 \( h_{S,L} = \ell^2(\Gamma_L) \) and \( h_{S,L} = -\Delta_L + v_L \), where \( \Delta_L u(x) = u(x-1) + u(x+1) \) is the discrete Laplacian on \( \Gamma_L \) with Dirichlet boundary conditions \( u(-1) = u(L+1) = 0 \) and \( v_L \) is the restriction of the potential \( v \) to \( \Gamma_L \). 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 \( \delta_x \) denotes the usual Kronecker delta at \( x \in \Gamma_L \). We denote by \( h_{T,L} \) the corresponding tunneling Hamiltonian and set
\[
h_L = h_{0,L} + h_{T,L}, \quad h_{0,L} = h_l \oplus h_{S,L} \oplus h_r.
\]
Denote by \( \varphi_{l/r,L}, \mathcal{J}_{l/r,L}, \) and \( \varsigma_L \) the spectral densities of the steady state fluxes and let
\[
\overline{\varsigma} = \{ E \mid \limsup_{L \to \infty} \varsigma_L(E) > 0 \},
\]
\[
\underline{\varsigma} = \{ E \mid \liminf_{L \to \infty} \varsigma_L(E) > 0 \}.
\]
Clearly, \( \underline{\varsigma} \subset \overline{\varsigma} \subset \Sigma_{l/r} \). Note also that
\[
\overline{\varsigma} = \{ E \mid \limsup_{L \to \infty} |\varphi_{l/r,L}(E)| > 0 \} = \{ E \mid \limsup_{L \to \infty} |\mathcal{J}_{l/r,L}(E)| > 0 \},
\]
and similarly for \( \underline{\varsigma} \).

Let \( h_S = -\Delta + v \) be the limiting half-line Schrödinger operator acting on \( \ell^2(\mathbb{Z}_+) \). If \( h_{S,L} \) is extended from \( \ell^2(\Gamma_L) \) to \( \ell^2(\mathbb{Z}_+) \) in the obvious way \( \text{by setting} \ h_{S,L} = 0 \text{on} \ \ell^2(\Gamma_L)^\perp \), then \( \lim_{L \to \infty} h_{S,L} = h_S \) in the strong resolvent sense. \( \delta_0 \) is a cyclic vector for \( h_S \) and the corresponding spectral measure \( \nu_S \) contains the full spectral information about \( h_S \). The set
\[
\Sigma_S = \left\{ E \mid \frac{d\nu_{S,ac}}{dE}(E) > 0 \right\},
\]
is the essential support of the absolutely continuous spectrum of \( h_S \). On physical grounds, it is natural to introduce:
**Property RST.** The half-line Schrödinger operator $h_S$ exhibits regular spectral transport if for any choice of the reservoirs $R_{l/r}$,

$$\Sigma = \mathcal{T} = \Sigma_S \cap \Sigma_{l/r}.$$  

(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 $\Sigma_S \subset \Sigma_{l/r}$, then $\Sigma_S$ 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 $B \subset \Sigma_S$ of positive Lebesgue measure,

$$\lim \inf_{L \to \infty} \int_B \varsigma_L(E)dE > 0,$$

while the dominated convergence theorem implies

$$\lim_{L \to \infty} \int_{B \setminus \Sigma_S} \varsigma_L(E)dE = 0.$$

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 $\mathcal{T}$ and $\mathcal{P}$ in terms of the growth of the norms of the transfer matrices associated to $h_S$. 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 $\varsigma_L$ 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

$$T_L(E) = \left[\begin{array}{cc} v(L) - E & -1 \\ 1 & 0 \end{array}\right] \cdots \left[\begin{array}{cc} v(0) - E & -1 \\ 1 & 0 \end{array}\right].$$

(1.13)

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

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

(1)

$$\lim_{k \to \infty} \varsigma_{L_k}(E) = 0.$$
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\[ \lim_{k \to \infty} \| T_{L_k}(E) \| = \infty. \]

Let

\[ \mathcal{S}_0 = \left\{ E \left| \sup_L \| T_L(E) \| < \infty \right\} \right., \quad \mathcal{S}_1 = \left\{ E \left| \lim_{L \to \infty} \| T_L(E) \| < \infty \right\} \right. \]

An immediate consequence of Theorem 1.3 is

**Corollary 1.4** (1)

\[ \mathcal{T} \equiv \mathcal{S}_0 \cap \Sigma_l \cap r. \]

(2)

\[ \mathcal{T} \equiv \mathcal{S}_1 \cap \Sigma_l \cap r. \]

(3) For any Borel set \( B \subset \mathcal{S}_0 \cap \Sigma_l \cap r \) of positive Lebesgue measure,

\[ \liminf_{L \to \infty} \int_B \varsigma_L(E) dE > 0. \]

(4)

\[ \lim_{L \to \infty} \int_{\mathbb{R} \setminus (\mathcal{S}_1 \cap \Sigma_l \cap r)} \varsigma_L(E) dE = 0. \]

It follows from Corollary 1.4 that Property RST is equivalent to

**Property SC.** \( \mathcal{S}_0 \equiv \Sigma_S \equiv \mathcal{S}_1. \)

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 the Schrödinger Conjecture. Regarding the existing results, the inclusion \( \mathcal{S}_0 \subset \Sigma_S \) was proven in [GP, KP] (see also [S2]). The inclusion \( \Sigma_S \subset \mathcal{S}_1 \) 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 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.

³We remark that to link Corollary 1.4 with transport in non-equilibrium statistical mechanics one needs that the Landauer-Büttiker formulæ 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 \( h_{l/r} = \ell^2(\mathbb{Z}_\pm), h_{l/r} = -k\Delta, k > 0. \) For other examples and general results regarding this point we refer the reader to [GJW].
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2 Proofs

2.1 Preliminaries

We will denote by $\text{sp}(A)$ the spectrum of a Hilbert space operator $A$, and write $\text{Im} \ A = (A - A^*)/2i$. If $A$ is self-adjoint, then $\text{sp}_{\text{ac}}(A)$ denotes its absolutely continuous spectrum and we write $A > 0$ whenever $\text{sp}(A) \subset [0, \infty]$. 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 $2 \times 2$ diagonal matrix with entries $F_{ab}(z) = \delta_{ab} F_a(z)$. We also introduce the $2 \times 2$ Green matrices $G^{(0)}_{ab,L}(z)$ and $G_{ab,L}(z)$ with entries

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

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 $H$ and $\psi_1, \psi_2 \in H$. For Lebesgue a.e. $E \in \mathbb{R}$ the boundary values

$$\langle \psi_1, (A - E - i0)^{-1} \psi_2 \rangle = \lim_{\varepsilon \downarrow 0} \langle \psi_1, (A - E - i\varepsilon)^{-1} \psi_2 \rangle,$$

exist and are finite. In the sequel, whenever we write $\langle \psi_1, (A - E - i0)^{-1} \psi_2 \rangle$, we will always assume that the limit exists and is finite. If the spectral measure $\nu_{\psi_1, \psi_2}$ for $A$ and $\psi_1, \psi_2$ is real-valued, then either $\psi_1$ is orthogonal to the cyclic subspace spanned by $A$ and $\psi_2$ and $\nu_{\psi_1, \psi_2}$ is the zero measure or $\langle \psi_1, (A - E - i0)^{-1} \psi_2 \rangle \neq 0$ for Lebesgue a.e. $E \in \mathbb{R}$. If $\psi \in \mathcal{F}$ then $\text{Im} \ \langle \psi, (A - E - i0)^{-1} \psi \rangle \geq 0$ and if $\nu_{\psi}$ is the spectral measure for $A$ and $\psi$, then

$$d\nu_{\psi, \text{ac}}(E) = \frac{1}{\pi} \text{Im} \ \langle \psi, (A - E - i0)^{-1} \psi \rangle dE,$$

so that the set $\{E \mid \text{Im} \ \langle \psi, (A - E - i0)^{-1} \psi \rangle > 0\}$ is an essential support of $\nu_{\psi, \text{ac}}$. In particular, one has

$$d\nu_{l/r, \text{ac}}(E) = \frac{1}{\pi} \text{Im} \ F_{l/r}(E + i0) dE,$$
and, with a slight abuse of notation, we may denote the following concrete representative of the class \( \Sigma_{l/r} \) by the same letter

\[
\{ E \mid \text{Im } F(E + i0) > 0 \} = \Sigma_{l/r}.
\]

In words, \( \Sigma_{l/r} \) consists of \( E \)’s for which the boundary values \( F_{l/r}(E + i0) \) 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

\[
t_L(E) = 2i(\text{Im } F(E + i0))^{1/2}G_L(E + i0)(\text{Im } F(E + i0))^{1/2}.
\]  
(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. \( E \in \mathbb{R} \),

\[
t_L^*(E)t_L(E) + t_L(E) + t_L^*(E) = 0.
\]  
(2.16)

It follows that

\[
\mathcal{R} = \mathcal{L} \{ E \in \Sigma_{l/r} \mid \text{Eqs. (2.15) and (2.16) hold} \},
\]

satisfies

\[
\Sigma_{l/r} \subseteq \mathcal{R}.
\]

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

**Lemma 2.1** For \( E \in \mathcal{R} \setminus \text{sp}(h_{S,L}) \), one has

\[
G_L^{(0)}(E) = (I - G_L^{(0)}(E)F(E + i0))G_L(E + i0).
\]

**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. \( \square \)

We proceed to relate the Green matrix \( G_L^{(0)} \) with the transfer matrix (1.13).
Lemma 2.2 For \( E \in \mathbb{R} \setminus \text{sp}(h_{S,L}) \) and any \( x, y, u, v \in \mathbb{C} \) one has

\[
G_L^{(0)}(E) \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} u \\ v \end{bmatrix} \iff T_L(E) \begin{bmatrix} u \\ x \end{bmatrix} = \begin{bmatrix} y \\ v \end{bmatrix}.
\]

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 \( E \in \mathbb{R} \setminus \text{sp}(h_{S,L}) \). For \( f \in \ell^2(\Gamma_L) \), the function \( \psi(x) = (\delta_x, (h_{S,L} - E)^{-1} f) \) satisfies the finite difference equation

\[
(-\Delta + v - E)\psi = f,
\]

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

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

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 \( G_L^{(0)}(E) \),

\[
T_L(E) \begin{bmatrix} G_{ll,L}^{(0)}(E) \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ G_{rr,L}^{(0)}(E) \end{bmatrix}, \quad T_L(E) \begin{bmatrix} G_{lr,L}^{(0)}(E) \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ G_{rr,L}^{(0)}(E) \end{bmatrix}.
\]

Thus, the two linearly independent vectors \((G_{ll,L}^{(0)}(E), 1, 0, G_{rr,L}^{(0)}(E))\) 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 \((1, 0, G_{ll,L}^{(0)}(E), G_{lr,L}^{(0)}(E))\) 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 \( G(E + i0) \).

Lemma 2.3 For \( E \in \mathbb{R} \setminus \text{sp}(h_{S,L}) \) and any \( x, y, u, v \in \mathbb{C} \) one has

\[
G_L(E + i0) \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} u \\ v \end{bmatrix} \iff T_L(E) \begin{bmatrix} u \\ x + F_l(E + i0)u \end{bmatrix} = \begin{bmatrix} y + F_r(E + i0)v \\ v \end{bmatrix}.
\]

In other words, the automorphism \( P : (x, y, u, v) \mapsto (u, x + F_l(E + i0)u, y + F_r(E + i0)v, v) \) of \( \mathbb{C}^4 \) maps the graph of \( G_L(E + i0) \) 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 $E \in \mathcal{R} \setminus (\bigcup_{L \in \mathcal{L}} \text{sp}(h_{S,L})) \cong \Sigma_{\Gamma_T}$ and $(L_k)_{k \in \mathbb{N}} \in \mathcal{L}$ be given. Then the following statements are equivalent.

(1) \[ \lim_{k \to \infty} G_{lr,L_k}(E + i0) = 0. \]

(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 $\|G_{L_k}(E + i0)\|$ is bounded. Writing

$$ G_{L_k}(E + i0) \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} u_k \\ v_k \end{bmatrix}, $$

we conclude that the sequences $u_k$ and $v_k$ are bounded while (1) implies $u_k = G_{lr,L_k}(E + i0) \to 0$. It follows from Lemma 2.3 that

$$ T_{L_k}(E) \begin{bmatrix} 1 \\ F_l(E + i0) \end{bmatrix} = \frac{1}{u_k} \begin{bmatrix} 1 + F_r(E + i0)v_k \\ v_k \end{bmatrix}, $$

which clearly implies (2).

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

$$ T_{L_k}(E) \begin{bmatrix} u_k \\ x_k + F_l(E + i0)u_k \end{bmatrix} = \begin{bmatrix} y_k + F_r(E + i0)v_k \\ v_k \end{bmatrix}, $$

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

$$ G_{L_k}(E + i0) \begin{bmatrix} x_k \\ y_k \end{bmatrix} = \begin{bmatrix} u_k \\ v_k \end{bmatrix}, $$

and the boundedness of $\|G_{L_k}(E + i0)\|$ 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

$$ G_{\Gamma_T}(E + i0) = \frac{u_k - G_{ll,L_k}(E + i0)x_k}{y_k}. $$

$\square$
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