

Landauer-Büttiker formula and Schrödinger conjecture

L. Bruneau¹, V. Jakšić², C.-A. Pillet³

¹ Département de Mathématiques and UMR 8088
CNRS and Université de Cergy-Pontoise
95000 Cergy-Pontoise, France

²Department of Mathematics and Statistics
McGill University
805 Sherbrooke Street West
Montreal, QC, H3A 2K6, Canada

³Aix-Marseille Univ, CPT, 13288 Marseille cedex 9, France
CNRS, UMR 7332, 13288 Marseille cedex 9, France
Univ Sud Toulon Var, CPT, B.P. 20132, 83957 La Garde cedex, France
FRUMAM

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 behavior of this steady state entropy flux in the limit $L \rightarrow \infty$ and relate persistence of transport to norm bounds on the transfer matrices of the limiting half-line Schrödinger operator $h_{\mathcal{S}}$. A natural conjecture is that the set of energies at which transport persists in the limit $L \rightarrow \infty$ is precisely the essential support of the absolutely continuous spectrum of $h_{\mathcal{S}}$. We show that this conjecture is equivalent to the Schrödinger conjecture in spectral theory of one-dimensional Schrödinger operators, thus giving a physically appealing interpretation to the Schrödinger conjecture.

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 $h = h_0 + h_T$, 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 $v : \mathbb{Z}_+ \rightarrow \mathbb{R}$ is a potential on the half line $\mathbb{Z}_+ = \{0, 1, \dots\}$. 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 $L \rightarrow \infty$ 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 $h_{\mathcal{S}} = -\Delta + v$ 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 $\psi \oplus 0$, $A \oplus 0$, \dots will be simply denoted by ψ , A , \dots . 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 $H_0 = d\Gamma(h_0)$, 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 $H_{l/r} = d\Gamma(h_{l/r})$ and $N_{l/r} = d\Gamma(1_{l/r})$.

¹We 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.

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

$$b_k^t(A) = e^{itd\Gamma(k)} A e^{-itd\Gamma(k)},$$

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

$$b_k^t(a^\#(f)) = e^{itd\Gamma(k)} a^\#(f) e^{-itd\Gamma(k)} = a^\#(e^{itk} f).$$

$\vartheta^t = b_1^t$ 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 $\tau_0^t = b_{h_0}^t$ preserves $\text{CAR}_\vartheta(\mathfrak{h})$ and describes the time evolution of the decoupled EBB model. The pair $(\text{CAR}_\vartheta(\mathfrak{h}), \tau_0^t)$ is a C^* -dynamical system.

For any self-adjoint operator ϱ 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 ω_ϱ on $\text{CAR}_\vartheta(\mathfrak{h})$. 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

$$\varrho_l \oplus \varrho_S \oplus \varrho_r,$$

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 ϱ_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 $\chi_{l/r} \in \mathfrak{h}_{l/r}$, $\psi_{l/r} \in \mathfrak{h}_S$. 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 $\tau^t = b_h^t$. 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 $\text{CAR}(\mathfrak{h})$, 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 $\text{CAR}_\vartheta(\mathfrak{h})$ for any $t \in \mathbb{R}$, and one easily verifies the relations

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

where

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

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

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

We recall the entropy balance equation [JP, Ru]

$$\text{Ent}(\omega_0 \circ \tau^t | \omega_0) = - \int_0^t \omega_0(\tau^s(\sigma)) ds, \quad (1.4)$$

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,

$$\frac{1}{t} \int_0^t \omega_0(\tau^s(\sigma)) ds \geq 0, \quad (1.5)$$

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 $t \rightarrow \infty$. To state the relevant result for the EBB model we need the assumption:

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

(A1) The single particle Hamiltonian h has no singular continuous spectrum.

Theorem 1.1 ([AJPP1]) *Suppose that (A1) holds. Then for all $A \in \text{CAR}_\vartheta(\mathfrak{h})$ the limit*

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

exists.

The functional ω_+ is a state on $\text{CAR}_\vartheta(\mathfrak{h})$ 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

$$\tilde{\mathfrak{h}} = \tilde{\mathfrak{h}}_l \oplus \mathfrak{h}_S \oplus \tilde{\mathfrak{h}}_r,$$

is invariant under h and h_0 , and $\Phi_{l/r}, \mathcal{J}_{l/r}, \sigma \in \text{CAR}_\vartheta(\tilde{\mathfrak{h}})$. 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 $\mathfrak{h}_{l/r} = L^2(\mathbb{R}, d\nu_{l/r})$, $\chi_{l/r}(E) = 1$ 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

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

where $\nu_{l/r,\text{ac}}$ is the absolutely continuous part of $\nu_{l/r}$ (w.r.t. Lebesgue measure). To avoid discussion of trivialities we shall always assume that $\nu_{l/r,\text{ac}}$ 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 $\nu_{l/r,\text{ac}}$, defined by,

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

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

$$B_1 \stackrel{\circ}{=} B_2 \Leftrightarrow |B_1 \triangle B_2| = 0,$$

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

$$w_{\pm} = \text{s-}\lim_{t \rightarrow \pm\infty} e^{ith} e^{-ith_0} 1_{\text{ac}}(h_0),$$

exist. The scattering matrix $s = w_+^* w_-$ is a unitary on $\mathfrak{h}_{\text{ac}}(h_0)$ 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)

$$\{E \mid \mathcal{T}(E) > 0\} \stackrel{\circ}{=} \Sigma_{l \cap r}. \quad (1.6)$$

Theorem 1.2 ([AJPP1]) *Suppose that (A1) holds. The steady state energy and charge currents are given by the following Landauer-Büttiker formulae*

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

where

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

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

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

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

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

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

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

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

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

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 (A1) 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 $v : \mathbb{Z}_+ \rightarrow \mathbb{R}$ 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 $\mathfrak{h}_{S,L} = \ell^2(\Gamma_L)$ and $h_{S,L} = -\Delta_L + v_L$, where $(\Delta_L u)(x) = u(x-1) + u(x+1)$ is the discrete Laplacian on 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

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

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

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

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

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

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

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 (by setting $h_{S,L} = 0$ on $\ell^2(\Gamma_L)^\perp$), then $\lim_{L \rightarrow \infty} h_{S,L} = h_S$

in the strong resolvent sense. δ_0 is a cyclic vector for h_S and the corresponding spectral measure ν_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 . Our work was motivated by the following

Conjecture 1. In the non-equilibrium case, for any choice of the reservoirs $\mathcal{R}_{l/r}$ and for any potential v ,

$$\underline{\Sigma} \stackrel{\circ}{=} \overline{\Sigma} \stackrel{\circ}{=} \Sigma_S \cap \Sigma_{l \cap r}. \quad (1.12)$$

This is a natural conjecture on physical grounds. If (A1) holds for all L and the reservoirs are chosen so that $\Sigma_S \subset \Sigma_{l \cap r}$, then Σ_S is precisely the set of energies at which transport persists in the limit $L \rightarrow \infty$. Moreover, by Fatou's lemma, for any Borel set $B \subset \Sigma_S$ of positive Lebesgue measure,

$$\liminf_{L \rightarrow \infty} \int_B \varsigma_L(E) dE > 0,$$

while the dominated convergence theorem implies

$$\lim_{L \rightarrow \infty} \int_{\mathbb{R} \setminus \Sigma_S} \varsigma_L(E) dE = 0.$$

Hence, the conjectured relation (1.12) would lead to a physically and mathematically very appealing characterization of the essential support of the absolutely continuous spectrum of half-line discrete Schrödinger operators.

We will not be able to settle Conjecture 1 in this paper. Our main result gives sharp characterizations of the sets $\overline{\Sigma}$ and $\underline{\Sigma}$ in terms of the growth of the norms of the transfer matrices associated to h_S . This characterization yields a partial result regarding Conjecture 1 and, combined with the results of Last-Simon [LS], shows that Conjecture 1 is equivalent to the so called Schrödinger conjecture (Conjecture 2 in the next section), which is considered by many as the most outstanding open problem in the spectral theory of one-dimensional Schrödinger operators³. This equivalence, which came as a surprise to us, sheds a light on the the Schrödinger conjecture and on 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

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

³We have made Conjecture 1 before we were aware of the Schrödinger conjecture.

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)

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

(2)

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

Let

$$\mathfrak{S}_0 = \left\{ E \mid \sup_L \|T_L(E)\| < \infty \right\}, \quad \mathfrak{S}_1 = \left\{ E \mid \liminf_{L \rightarrow \infty} \|T_L(E)\| < \infty \right\}.$$

An immediate consequence of Theorem 1.3 is

Corollary 1.4 (1)

$$\mathfrak{I} \doteq \mathfrak{S}_0 \cap \Sigma_{l \cap r}.$$

(2)

$$\overline{\mathfrak{I}} \doteq \mathfrak{S}_1 \cap \Sigma_{l \cap r}.$$

(3) *For any Borel set $B \subset \mathfrak{S}_0 \cap \Sigma_{l \cap r}$ of positive Lebesgue measure,*

$$\liminf_{L \rightarrow \infty} \int_B \varsigma_L(E) dE > 0.$$

(4)

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

It follows from fundamental results of Last and Simon (Theorems 1.1 and 1.2 in [LS]) that

$$\mathfrak{S}_0 \subset \Sigma_S \subset \mathfrak{S}_1,$$

and so, by Corollary 1.4, Conjecture 1 is equivalent to

Conjecture 2. $\mathfrak{S}_0 \doteq \Sigma_S \doteq \mathfrak{S}_1$.

We have learned from Yoram Last that Conjecture 2 is a fundamental open problem in the theory of one dimensional Schrödinger operators, known as the Schrödinger Conjecture (see [MMG] and Appendix C4 in [S]). It is widely believed that this conjecture holds for all potentials v .

Theorem 1.3 and Corollary 1.4 reformulate the Schrödinger conjecture, via the Landauer-Büttiker formula, in terms of non-equilibrium transport and shed a new light on its physical interpretation.⁴ The conjecture appears very natural from the point of view of transport theory and its failure would provide examples of models with strikingly singular non-equilibrium transport on a set of energies of positive Lebesgue measure.

Acknowledgment. The research of L.B. and C.-A.P. was partly supported by ANR (grant 09-BLAN-0098). The research of V.J. was partly supported by NSERC. A part of this work was done during the visit of the first author to McGill University supported by NSERC. Another part was done during the stay of the second author at University of Cergy-Pontoise. V.J. wishes to thank V. Georgescu and F. Germinet for making this visit possible and for their hospitality. We wish to thank Y. Last for useful discussions.

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 $a, b, c, \dots \in \{l, r\}$. 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

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

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

$$\langle \psi_1, (A - E - i0)^{-1} \psi_2 \rangle = \lim_{\epsilon \downarrow 0} \langle \psi_1, (A - E - i\epsilon)^{-1} \psi_2 \rangle, \quad (2.14)$$

exists 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 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

⁴We 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].

$\langle \psi_1, (A - E - i0)^{-1} \psi_2 \rangle \neq 0$ for Lebesgue a.e. $E \in \mathbb{R}$. If $\psi \in \mathfrak{H}$ then $\text{Im} \langle \psi, (A - E - i0)^{-1} \psi \rangle \geq 0$ and if ν_ψ is the spectral measure for A and ψ , then

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

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

In particular, one has

$$d\nu_{l/r,ac}(E) = \frac{1}{\pi} \text{Im} F_{l/r}(E + i0) dE,$$

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

$$\{E \mid \text{Im} F(E + i0) > 0\} = \Sigma_{l \cap r}.$$

In words, $\Sigma_{l \cap r}$ 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

$$t_L(E) = 2i(\text{Im} F(E + i0))^{1/2} G_L(E + i0) (\text{Im} F(E + i0))^{1/2}. \quad (2.15)$$

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. $E \in \mathbb{R}$,

$$t_L^*(E) t_L(E) + t_L(E) + t_L^*(E) = 0. \quad (2.16)$$

It follows that

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

satisfies

$$\Sigma_{l \cap r} \doteq \mathfrak{R}.$$

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

Lemma 2.1 For $E \in \mathfrak{R} \setminus \text{sp}(h_{S,L})$, 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 $\psi(x) = \langle \delta_x, (h_{S,L} - E)^{-1} f \rangle$ satisfies the finite difference equation

$$(-\Delta + v - E)\psi = f, \quad (2.17)$$

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

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

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

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

Thus, the two linearly independent vectors $(G_{ul,L}^{(0)}(E), 1, 0, G_{rl,L}^{(0)}(E))$ 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 $(1, 0, G_{ul,L}^{(0)}(E), G_{rl,L}^{(0)}(E))$ and $(0, 1, G_{lr,L}^{(0)}(E), G_{rr,L}^{(0)}(E))$ which span the graph of $G_L^{(0)}(E)$. \square

Combining the two previous lemmata, we obtain the connection between the transfer matrix and the Green matrix $G(E + i0)$.

Lemma 2.3 For $E \in \mathfrak{R} \setminus \text{sp}(h_{S,L})$ 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 $E \in \mathfrak{R} \setminus (\cup_L \text{sp}(h_{S,L})) \stackrel{\circ}{=} \Sigma_{l \cap r}$ and $(L_k)_{k \in \mathbb{N}} \in \mathfrak{L}$ be given. Then the following statements are equivalent.

(1)

$$\lim_{k \rightarrow \infty} G_{lr, L_k}(E + i0) = 0.$$

(2)

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

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 $u_k = G_{lr, L_k}(E + i0) \rightarrow 0$. 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 $|v_k| + |y_k|$ 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 $|y_k| \rightarrow \infty$ and (1) follows from

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

□

References

- [Ar] Araki, H.: Relative entropy of states of von Neumann algebras. *Publ. Res. Inst. Math. Sci. Kyoto Univ.* **11**, 809 (1975/76).
- [AJPP1] Aschbacher, W., Jakšić, V., Pautrat, Y., Pillet, C.-A.: Transport properties of quasi-free fermions. *J. Math. Phys.* **48**, 032101 (2007).
- [AJPP2] Aschbacher, W., Jakšić, V., Pautrat, Y., Pillet, C.-A.: Topics in non-equilibrium quantum statistical mechanics. In *Open Quantum System III. Recent Developments*. S. Attal, A. Joye and C.-A. Pillet editors. *Lecture Notes in Mathematics* **1882**, 1, Springer, New York, 2006.
- [GJW] Grech, P., Jakšić, V., Westrich M.: In preparation.
- [J] Jakšić, V.: Topics in spectral theory. In *Open Quantum Systems I. The Hamiltonian Approach*. S. Attal, A. Joye and C.-A. Pillet editors. *Lecture Notes in Mathematics* **1880**, 235, Springer, New York, 2006.
- [JKP] Jakšić, V., Kritchevski, E., Pillet, C.-A.: Mathematical theory of the Wigner-Weisskopf atom. In *Large Coulomb systems*. J. Dereziński and H. Siedentop editors. *Lecture Notes in Physics* **695**, 145, Springer, New York, 2006.
- [JP] Jakšić, V., Pillet, C.-A.: On entropy production in quantum statistical mechanics. *Commun. Math. Phys.* **217**, 285 (2001).
- [LS] Last, Y., Simon, B.: Eigenfunctions, transfer matrices, and absolutely continuous spectrum of one-dimensional Schrödinger operators. *Invent. Math.* **135**, 329 (1999).
- [MMG] Maslov, V.P., Molchanov, S.A., Gordon, A. Ya.: Behavior of generalized eigenfunctions at infinity and the Schrödinger conjecture. *Russian J. Math. Phys.* **1**, 71 (1993).
- [N] Nenciu, G.: Independent electrons model for open quantum systems: Landauer-Büttiker formula and strict positivity of the entropy production. *J. Math. Phys.* **48**, 033302 (2007).
- [Ru] Ruelle, D.: Entropy production in quantum spin systems. *Commun. Math. Phys.* **224**, 3 (2001).
- [S] Simon, B.: Schrödinger semigroups. *Bulletin AMS* **7**, 447 (1982).
- [Y] Yafaev, D.R.: *Mathematical scattering theory. General theory*. Translated from the Russian by J. R. Schulenberger. *Translations of Mathematical Monographs* **105**. American Mathematical Society, Providence, RI, 1992.