What is absolutely continuous spectrum?

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Abstract. We characterize the absolutely continuous spectrum of half-line Jacobi matrices in terms of electronic transport in a suitable class of open quantum systems.

1 Introduction

Spectral types (e.g., pure point, singular continuous, absolutely continuous) of self-adjoint operators are completely characterized in terms of the boundary values of the resolvent. Dynamical characterizations, linking spectral types to physical properties of the corresponding quantum systems, are more subtle. In this note, we focus on the well established heuristics that the ac spectrum of a quantum Hamiltonian is the set of energies at which the described system exhibits transport. Much effort has been devoted to the investigation of these heuristics; so far many results many results have been unfavorable.

In this note we consider bounded half-line Jacobi matrices, operators of the form

$$(Ju)(n) = a_n u(n+1) + b_n u(n) + a_{n-1} u(n-1)$$

acting on $\ell^2(\mathbb{N})$ with boundary condition $u(0) = 0$ and where $(a_n)_n$, $(b_n)_n$ are bounded sequences with $a_n > 0$. The usual discrete Schrödinger operators correspond to $a_n \equiv 1$. The case of a general bounded self-adjoint operator H is considered in an expanded version of this note [7].

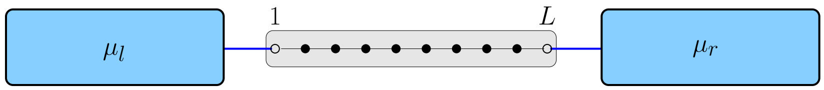

Figure 1: A finite sample of length L coupled to two electronic reservoirs.

In large part, the main novelty of our approach is due to the use of an appropriate notion of transport. The latter is usually related, at least in the mathematics literature, to the properties of the unitary group $\mathrm{e}^{-\mathrm{i}tJ}$. Detailed studies of the link between dynamics, transport, and spectrum revealed an intricate complex dependence that is only partially understood, many basic questions remaining open.

Our approach can be described as follows. One constructs a family of Electronic Black Box models[1] indexed by $L \in \mathbb{N}$: two electronic reservoirs are attached at the end points of the finite sample obtained by restricting J to the interval $Z_L = \{1, \cdots, L\}$, see Figure 1. The left/right electronic reservoir is at zero temperature and chemical potential μ_l/μ_r, where $\mu_r > \mu_l$, while the Hamiltonian of the sample is the restriction of J to Z_L. The voltage differential $\mu_r - \mu_l$ generates an electronic current between the reservoirs. The steady state value $\langle \mathcal{J}_L \rangle_+$ of this current is given by the celebrated Landauer-Büttiker formula. Our approach to the *ac spectrum/transport* duality relates the energies in the ac spectrum of the operator J in the interval $]\mu_l, \mu_r[$ to the energies at which the current $\langle \mathcal{J}_L \rangle_+$ persists in the limit $L \to \infty$. This naturally leads to the *Absolutely Continuous Spectrum–Electronic Transport Conjecture* (abbreviated ACET) that these two sets of energies coincide; see Section 4.

In the physics literature this approach can be traced back to the 1970's and to pioneering works on the conductance of 1D samples by Landauer, Büttiker, Thouless, Anderson, Lee, and many others. Until recently, however, mathematically rigorous proofs of the transport formulas proposed by physicists were not available, hampering mathematical development. Recent proofs of the Landauer-Büttiker and Thouless formulas from the first principles of quantum mechanics [2, 11, 4] have opened the way for a systematic study of the proposed approach.

One surprising outcome is the fact that the ACET Conjecture is essentially equivalent to the celebrated *Schrödinger Conjecture*, which states that the generalized eigenfunctions of J are bounded for almost all energies in the essential support of the ac spectrum. The announcement of this equivalence in [3], which has given a somewhat surprising physical interpretation to the Schrödinger Conjecture in terms of electronic transport, coincided with Avila's announcement of a counterexample to the Schrödinger Conjecture [1]. For many years, the latter was regarded as the single most important open problem in the spectral theory of Schrödinger operators. Its failure induced that of the ACET Conjecture and thus had direct physical implications. These developments have lead to a weaker form of these conjectures which were stated and proven in [5, 6]; see Section 5.

2 Schrödinger Conjectures

Let ν be the spectral measure of J for δ_1[2]. Since δ_1 is cyclic for J, ν encodes all the spectral properties of J. Fixing $E \in \mathbb{R}$, let $u_E = (u_E(n))_n$ be the unique solution of the stationary Schrödinger equation

[1] EBB models are always understood in the independent electrons approximation.
[2] $\{\delta_n\}_{n\geq 1}$ denotes the standard basis of $\ell^2(\mathbb{N})$.

$Ju_E = Eu_E$ satisfying $u_E(0) = 0$, $u_E(1) = 1$. The following well-known bound holds:[3] for any $\epsilon > 0$ and for ν–a.e. E there is a finite constant $C_{E,\epsilon} > 0$ such that, for all $n \geq 1$, $|u_E(n)| \leq C_{E,\epsilon} n^{1/2+\epsilon}$.

The Schrödinger Conjectures are deep refinements of this simple bound. In a nutshell, they state that the generalized eigenfunctions $u_E(n)$ are bounded for an appropriate set of energies E. These conjectures are rooted in formal computations and implicit assumptions by physicists. Their formulation has evolved over time, and they are linked to conjectures that have appeared independently in the mathematical literature, such as the Steklov Conjecture [12, 15].

The Schrödinger Conjecture for the pure point spectrum is trivial. The Schrödinger Conjecture for the singular continuous spectrum asserts that for all Jacobi matrices J, $\sup_{n\geq 1} |u_E(n)| < \infty$ for ν_{sing}-a.e. E. A counterexample to this conjecture was found by Jitomirskaya [9]. This leaves us with the Schrödinger Conjecture for the absolutely continuous spectrum which states that for all Jacobi matrices J, $\sup_{n\geq 1} |u_E(n)| < \infty$ for ν_{ac}-a.e. E. In terms of the transfer matrices[4]

$$T_E(n) = A_E(n) \cdots A_E(1), \qquad A_E(x) = a_x^{-1} \begin{bmatrix} E - b_x & -1 \\ a_x^2 & 0 \end{bmatrix},$$

and using the invariance of ac spectrum under rank one perturbations[5], one arrives at the equivalent formulation

Schrödinger Conjecture I. For all Jacobi matrices J and $E \in \Sigma_{\text{ac}}(J)$,[6]

$$\sup_{n\geq 1} \|T_E(n)\| < \infty.$$

Among other partial results toward this conjecture, Gilbert and Pearson [8] (see also [13]) showed that

$$\{E \mid \sup_{n\geq 1} \|T_E(n)\| < \infty\} \subset \Sigma_{\text{ac}}(J).$$

The normalization $\int_{\mathbb{R}} \|u_E(n)|^2 \mathrm{d}\nu(E) = 1$ and Fatou's Lemma give

$$\Sigma_{\text{ac}}(J) \subset \{E \mid \liminf_{n\to\infty} \|T_E(n)\| < \infty\}. \tag{2.1}$$

Last and Simon [10] refined (2.1) and established the averaged form of the Conjecture:

$$\Sigma_{\text{ac}}(J) = \left\{ E \mid \liminf_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \|T_E(n)\|^2 < \infty \right\}.$$

[3] For $f \in \ell^2(\mathbb{N})$, $\|f\|^2 = \sum_{n\geq 1} |f(n)|^2 = \sum_{n\geq 1} |f(n)|^2 \int_{\mathbb{R}} |u_E(n)|^2 \mathrm{d}\nu(E)$. The estimate follows by taking $f(n) = |n|^{-1/2-\epsilon}$ and applying Fubini's theorem.

[4] Note that u_E is a solution of the eigenvalue equation iff $\begin{bmatrix} u_E(n+1) \\ a_n u_E(n) \end{bmatrix} = A_E(n) \begin{bmatrix} u_E(n) \\ a_{n-1} u_E(n-1) \end{bmatrix}$.

[5] In other words, to show that the new formulation implies the original, one also considers the conjecture for $J_\theta := J + \theta|\delta_1\rangle\langle\delta_1|$. In this case, $\Sigma_{\text{ac}}(J_\theta) = \Sigma_{\text{ac}}(J)$ and $u_{\theta,E}$ satisfy $Eu_{\theta,E} = Ju_{\theta,E}$ with boundary condition $u_{\theta,E}(0) = \theta$, $u_{\theta,E}(1) = 1$. Since $\begin{bmatrix} u_{E,\theta}(n+1) \\ a_n u_{E,\theta}(n) \end{bmatrix} = T_E(n) \begin{bmatrix} 1 \\ \theta \end{bmatrix}$, and $\mathrm{sp}_{\text{ac}}(J) = \emptyset$ if $\liminf a_n = 0$, the Schrödinger Conjecture for two different θ's gives $\sup_{n\geq 1} \|T_E(n)\| < \infty$.

[6] $\Sigma_{\text{ac}}(J)$ denotes the essential support of the ac spectrum of J.

A particularly striking aspect of Avila's counterexample [1] to the Schrödinger Conjecture I is that it concerns a spectrally rigid[7] class of Jacobi matrices describing discrete ergodic Schrödinger operators. In this setting $a_n \equiv 1$ and $b_\omega(n) = B(S^n\omega)$, $\omega \in \Omega$, where Ω is a probability space, $B : \Omega \to \mathbb{R}$ is a bounded measurable map, and S is an ergodic invertible transformation of Ω. The ergodicity gives that there are deterministic sets $\Sigma_{\rm ac}$ and $\mathcal{B}$ such that for a.e. $\omega \in \Omega$, $\Sigma_{\rm ac} = \Sigma_{\rm ac}(J_\omega)$, $\mathcal{B} = \{E \,|\, \sup_{n\geq 1} \|T_E(\omega, n)\| < \infty\}$. Avila constructs Ω, B, and an ergodic transformation S such that the set $\Sigma_{\rm ac} \setminus \mathcal{B}$ has strictly positive Lebesgue measure.

The following variant of the Schrödinger Conjecture was motivated by the the ACET Conjecture which we will discuss in Section 4:

Schrödinger Conjecture II. For all Jacobi matrices J,

$$\Sigma_{\rm ac}(J) = \{E \,|\, \liminf_{n\to\infty} \|T_E(n)\| < \infty\}.$$

The Kotani theory [14] gives that Conjecture II holds for discrete *ergodic* Schrödinger operators. The validity of this conjecture for general J remains an open problem. The following weak form of Conjectures I and II was formulated and proved in [5]:

Theorem 2.1 *For any Jacobi matrix J, any interval $]a, b[$, and any sequence of integers $L_n \to \infty$ one has*

$$\mathrm{sp}_{\rm ac}(J)\cap]a, b[= \emptyset \quad \Longleftrightarrow \quad \lim_{n\to\infty} \int_a^b \|T_E(L_n)\|^{-2} \mathrm{d}E = 0.$$

This result plays a key role in the characterization of the ac spectrum by transport properties; see Section 5.

3 Landauer-Büttiker formula

To a Jacobi matrix J we associate the following EBB models. For $L \geq 1$, the finite sample is described by the one-particle Hilbert space $\mathcal{H}_L = \ell^2(Z_L)$, $Z_L = \{1, \cdots, L\}$, and the one-particle Hamiltonian J_L, the restriction of J to Z_L with Dirichlet b.c. The left/right electronic reservoir $\mathcal{R}_{l/r}$ is described by the spectral triple $(\mathcal{H}_{l/r}, H_{l/r}, \psi_{l/r})$, where $\psi_{l/r}$ is a unit vector cyclic for $H_{l/r}$. The one-particle Hilbert space of the joint system reservoirs + sample is $\mathcal{H} = \mathcal{H}_l \oplus \mathcal{H}_L \oplus \mathcal{H}_r$ and its one-particle Hamiltonian is $H_\lambda = H_0 + \lambda V$, where $H_0 = H_l \oplus J_L \oplus H_r$,

$$V := |\delta_1\rangle\langle\psi_l| + |\psi_l\rangle\langle\delta_1| + |\delta_L\rangle\langle\psi_r| + |\delta_L\rangle\langle\psi_r|,$$

and $\lambda \neq 0$ is a coupling constant. The full Hilbert space of the joint system is the anti-symmetric Fock space $\mathcal{F}$ over $\mathcal{H}$ and its full Hamiltonian is the second quantization $\mathrm{d}\Gamma(H_\lambda)$ of H_λ. The observables of the joint system are elements of the C^*-algebra $\mathcal{O}$ of bounded operators on $\mathcal{F}$ generated by $\mathbb{1}$ and the family $\{a^*(f)a(g) \,|\, f, g \in \mathcal{H}\}$, where a^*/a are the creation/annihilation operators on $\mathcal{F}$. The electronic current observable is

$$\mathcal{J}_L := -\mathrm{i}\lambda \mathrm{d}\Gamma([V, \mathbb{1}_r]),$$

[7]The rigidity here refers to Kotani theory [14].

where $\mathbb{1}_r$ is the orthogonal projection from $\mathcal{H}$ onto $\mathcal{H}_r$. We assume that the l/r reservoir is initially at zero temperature and chemical potential $\mu_{l/r}$, where $\mu_r > \mu_l$, while the sample is in an arbitrary state. More precisely, the initial state of system is the quasi-free state ω_{μ_l,μ_r} on $\mathcal{O}$ generated by $T = T_l \oplus T_L \oplus T_r$, where $T_{l/r}$ is the spectral projection of $H_{l/r}$ onto the interval $]-\infty, \mu_{l/r}]$ and for definiteness $T_L = \mathbb{1}_L/L$, where $\mathbb{1}_L$ is the orthogonal projection from $\mathcal{H}$ onto $\mathcal{H}_L$. The chemical potential difference generates an electronic current from the right to the left reservoir across the sample whose expectation value at time t is

$$\langle \mathcal{J}_L \rangle_t = \omega_{\mu_l,\mu_r}\left(\mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma(H_\lambda)} \mathcal{J}_L \mathrm{e}^{-\mathrm{i}t\mathrm{d}\Gamma(H_\lambda)}\right).$$

Assuming that H_λ has no singular continuous spectrum, one proves [2, 11]

$$\langle \mathcal{J} \rangle_+(L) := \lim_{t\to\infty} \frac{1}{t}\int_0^t \langle \mathcal{J}_L \rangle_s \mathrm{d}s = \frac{1}{2\pi}\int_{\mu_l}^{\mu_r} \mathcal{D}(L, E)\mathrm{d}E, \tag{3.1}$$

where

$$\mathcal{D}(L, E) = 4\pi^2\lambda^4 |\langle \delta_1, (H_\lambda - E - \mathrm{i}0)^{-1}\delta_L\rangle|^2 \frac{\mathrm{d}\nu_{l,\mathrm{ac}}}{\mathrm{d}E}(E)\frac{\mathrm{d}\nu_{r,\mathrm{ac}}}{\mathrm{d}E}(E) \tag{3.2}$$

is the one-particle transmittance ($\nu_{l/r}$ being the spectral measure of $H_{l/r}$ for $\psi_{l/r}$). Relations (3.1) and (3.2) constitute the Landauer-Büttiker formula. We emphasize that its derivation is dynamical and based on the first principles of quantum mechanics.

Note that $\Sigma_{\mathrm{ac},l/r} := \{E \,|\, \frac{\mathrm{d}\nu_{l/r,\mathrm{ac}}}{\mathrm{d}E}(E) > 0\}$ is the essential support of the ac spectrum of $H_{l/r}$. To avoid discussion of trivialities, in what follows we shall assume that the reservoirs are chosen so that $\Sigma_{\mathrm{ac}}(J) \subset \Sigma_{\mathrm{ac},l/r}$.

4 Linear response and Schrödinger Conjectures

Setting $\mu_l = \mu$, $\mu_r = \mu + \epsilon$, the Landauer-Büttiker formula gives

$$\mathcal{L}_L(\mu) := \lim_{\epsilon\downarrow 0} \frac{1}{\epsilon}\langle \mathcal{J}_L \rangle_+ = \frac{1}{2\pi}\mathcal{D}(L, \mu), \quad \text{for Lebesgue a.e. } \mu.$$

The starting point of our research program was the conjecture that the linear response conductance $\mathcal{L}_L$ characterizes $\Sigma_{\mathrm{ac}}(J)$. More precisely, let

$$\overline{\mathcal{T}} := \{\mu \,|\, \limsup_{L\to\infty} \mathcal{L}_L(\mu) > 0\}, \qquad \underline{\mathcal{T}} := \{\mu \,|\, \liminf_{L\to\infty} \mathcal{L}_L(\mu) > 0\}.$$

The following conjecture was made in the preprint version of [3], prior to Avila's announcement of the results [1]:

> **ACET Conjecture.** For all Jacobi matrices J, $\underline{\mathcal{T}} = \overline{\mathcal{T}} = \Sigma_{\mathrm{ac}}(J)$.

The main result of [3] are the relations

$$\underline{\mathcal{T}} = \{E \,|\, \sup_{n\geq 1} \|T_E(n)\| < \infty\}, \qquad \overline{\mathcal{T}} = \{E \,|\, \liminf_{n\to\infty} \|T_E(n)\| < \infty\},$$

which show that the ACET Conjecture is equivalent to the Schrödinger Conjectures I+II. Avila's counterexample disproves the part $\underline{\mathcal{T}} = \Sigma_{\mathrm{ac}}(J)$, while the validity of $\overline{\mathcal{T}} = \Sigma_{\mathrm{ac}}(J)$ for all Jacobi matrices remains an open problem.

5 Characterization of the absolutely continuous spectrum

5.1 Landauer-Büttiker transport

Physically, the message conveyed by Avila's counterexample is that the Landauer-Büttiker linear response fails to characterize the essential support of the ac spectrum. By contrast, [5] shows that the large L asymptotics of the steady state current fully characterize the absolutely continuous spectrum.

Theorem 5.1 *For any Jacobi matrix J, any $\mu_r > \mu_l$, all reservoirs satisfying $]\mu_l, \mu_r[\subset \Sigma_{\mathrm{ac},l/r}$, and any sequence of integers $L_n \to \infty$, one has*

$$\mathrm{sp}_{\mathrm{ac}}(J) \cap]\mu_l, \mu_r[= \emptyset \quad \Longleftrightarrow \quad \lim_{n\to\infty} \langle \mathcal{J}_{L_n} \rangle_+ = 0.$$

The proof proceeds by showing that $\lim \langle \mathcal{J}_{L_n} \rangle_+ = 0 \Leftrightarrow \lim \int_{\mu_l}^{\mu_r} \|T_E(L_n)\|^{-2} \mathrm{d}E = 0$ and by invoking Theorem 2.1.

5.2 Thouless transport

The Thouless formula is a special case of the Landauer-Büttiker formula in which the reservoirs are implemented such that the coupled Hamiltonian H_λ is a periodic Jacobi matrix. More precisely, let $J_{L,\mathrm{per}}$ be the periodic Jacobi matrix on $\ell^2(\mathbb{Z})$ obtained by extending the Jacobi parameters $(a_n)_{1\le n<L}$ and $(b_n)_{1\le n\le L}$ of the sample Hamiltonian J_L by setting $a_L = \lambda_{\mathcal{S}}$ and

$$a_{x+nL} = a_x, \qquad b_{x+nL} = b_x, \qquad n \in \mathbb{Z},\ x \in Z_L.$$

The internal coupling constant $\lambda_{\mathcal{S}} \neq 0$ is a priori an arbitrary parameter. The one-particle Hilbert spaces of the reservoirs are $\mathcal{H}_l = \ell^2(] - \infty, 0] \cap \mathbb{Z})$ and $\mathcal{H}_r = \ell^2([L+1, \infty[\cap \mathbb{Z})$; the corresponding one-particle Hamiltonians are the restriction, with Dirichlet boundary condition, of $J_{L,\mathrm{per}}$ to $] - \infty, 0] \cap \mathbb{Z}$ and $[L+1, \infty[\cap \mathbb{Z}$ respectively. Finally, $\psi_l = \delta_0$, $\psi_r = \delta_{L+1}$, and the coupling constant is set to $\lambda = \lambda_{\mathcal{S}}$. For such EBB models the Landauer-Büttiker formula coincides with the Thouless formula:

$$\langle \mathcal{J}_L^{\mathrm{Th}} \rangle_+ = |\mathrm{sp}(J_{L,\mathrm{per}}) \cap]\mu_l, \mu_r[| \,, \tag{5.1}$$

where $|\cdot|$ denotes Lebesgue measure. For Thouless transport we also have [5]

Theorem 5.2 *For any Jacobi matrix J, any $\mu_r > \mu_l$ and any sequence of integers $L_n \to \infty$ one has*

$$\mathrm{sp}_{\mathrm{ac}}(J) \cap]\mu_l, \mu_r[= \emptyset \quad \Longleftrightarrow \quad \lim_{n\to\infty} \langle \mathcal{J}_{L_n}^{\mathrm{Th}} \rangle_+ = 0.$$

The proof proceeds by showing that $\lim \langle \mathcal{J}_{L_n}^{\mathrm{Th}} \rangle_+ = 0 \Leftrightarrow \lim \int_{\mu_l}^{\mu_r} \|T_E(L_n)\|^{-2} \mathrm{d}E = 0$. The details of the proof, however, are considerably more involved than in the case of Theorem 5.1.

Remark. A third notion of electronic transport, called Crystalline transport, was introduced in [4] as a link between the Landauer-Büttiker and Thouless transport. It is shown in [6] that this crystalline transport also fully characterizes the ac spectrum. We refer the reader to the original papers [4, 6] and to the expanded version of this note [7] for more details about this notion.

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