What is absolutely continuous spectrum?

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Abstract. This note is an expanded version of the authors' contribution to the Proceedings of the ICMP Santiago, 2015, and is based on a talk given by the second author at the same Congress. It concerns a research program [BJP, BJLP1, BJLP2, BJLP3] devoted to the characterization of the absolutely continuous spectrum of a self-adjoint operator H in terms of the transport properties of a suitable class of open quantum systems canonically associated to H.

1 Introduction

Early developments of the mathematical foundations and axiomatizations of non-relativistic quantum mechanics naturally led to the formulation and proof of the spectral theorem for self-adjoint operators [Neu]. Ever since, many of the developments in spectral theory were inspired by this link. The question we address here concerns the characterization of spectral types (e.g.– pure point, singular continuous, absolutely continuous). Although these spectral types are completely determined by the boundary values of the resolvent, their dynamical characterizations in terms of the physical properties of the corresponding quantum systems are more subtle. We shall focus on the well established heuristic that

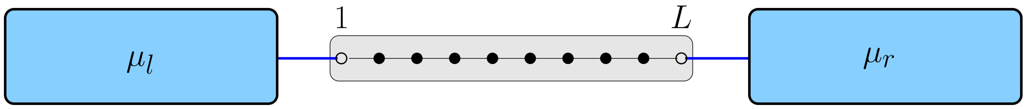

Figure 1: A finite sample of length L coupled to two electronic reservoirs

the absolutely continuous (ac) spectrum of a quantum Hamiltonian is the set of energies at which the described physical system exhibits transport. Much effort has been devoted to the investigation of this heuristic; so far many results have been unfavorable.

The basic unit of spectral theory is a *spectral triple* $(\mathcal{H}, H, \psi)$ where $\mathcal{H}$ is a Hilbert space,[1] H is a bounded self-adjoint operator on $\mathcal{H}$, and $\psi \in \mathcal{H}$ is a unit vector cyclic for H.[2] The transport properties of $(\mathcal{H}, H, \psi)$ are usually defined and analyzed, at least in the mathematics literature, through the properties of the unitary group $\mathrm{e}^{-\mathrm{i}tH}$ which defines the quantum dynamics generated by H; see Section 2.

In large part, the novelty of our approach is the use of an appropriate notion of transport which can be briefly described as follows. The abstract triple $(\mathcal{H}, H, \psi)$ is canonically identified with a triple $(\ell^2(\mathbb{N}), J, \delta_1)$, where J is a Jacobi matrix and $\{\delta_n\}_{n\geq 1}$ denotes the standard basis of $\ell^2(\mathbb{N})$; see Section 3. Once such an identification is made, one constructs a family of Electronic Black Box (EBB) models[3] indexed by $L \in \mathbb{N}$ as follows: two electronic reservoirs are attached at the end points of a finite sample obtained by restricting J to the interval $Z_L = \{1, \ldots, L\}$; 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 operator J restricted to Z_L. The voltage differential $\mu_r - \mu_l$ generates an electronic current from the right to the left reservoir whose steady state value $\langle \mathcal{J}_L \rangle_+$ is given by the celebrated Landauer-Büttiker formula; see Section 5. Our approach to the *ac spectrum/transport* duality is to relate the energies in the absolutely continuous 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 6.

In the physics literature the proposed 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 [AJPP, N, BJLP1] have opened the way to systematic studies of the proposed approach.

One surprising outcome of this study is the realization 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 absolutely continuous spectrum. The announcement of this equivalence in [BJP], which has given a surprising physical interpretation to the Schrödinger Conjecture in terms of the electronic transport, coincided with Avila's announcement of a counterexample to the Schrödinger Conjecture [Av]. For many years the Schrödinger Conjecture was

[1] To avoid discussion of, for our purposes, trivial cases, we shall always assume that $\dim \mathcal{H} = \infty$.

[2] The vector ψ is cyclic for H iff the linear span of the set $\{H^n\psi \,|\, n \geq 0\}$ is dense in $\mathcal{H}$.

[3] These models are always considered in the independent electrons approximation.

regarded as the single most important open problem in the general spectral theory of Schrödinger operators. Its failure induced that of the ACET Conjecture and thus had direct physical implications. These developments have led to a weaker form of the conjectures, stated and proven in [BJLP2, BJLP3].

This note is organized as follows. In Section 2 we fix the notation and review the resolvent approach to the spectral theorem. The Jacobi matrix representation of a spectral triple is described in Section 3. The Schrödinger Conjectures are reviewed in Section 4. The Electronic Black Box models associated to the Jacobi matrix representation, the Landauer-Büttiker formula, and the ACET Conjecture of [BJP] are described in Sections 5 and 6. The results of [BJLP1, BJLP2, BJLP3] are described in 7. The concluding remarks, including a brief discussion of future research directions, are presented in Section 8.

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2 Spectral triples and the spectral theorem

In this section we briefly review the resolvent approach to the spectral theorem. A more detailed exposition of these results can be found in [J].

Given the spectral triple $(\mathcal{H}, H, \psi)$, the Poisson representation of positive harmonic functions yields a unique Borel probability measure ν on $\mathbb{R}$ such that, for all z in the open half-plane $\mathbb{C}_+ = \{z \in \mathbb{C} \,|\, \mathrm{Im}\,(z) > 0\}$,

$$F(z) := \langle \psi, (H - z)^{-1} \psi \rangle = \int_{\mathbb{R}} \frac{\mathrm{d}\nu(E)}{E - z}. \tag{2.1}$$

ν is the spectral measure for H and ψ and the function F is its Borel transform. The representation (2.1) easily yields the spectral theorem in its basic form: there exists a unitary operator $U : \mathcal{H} \to L^2(\mathbb{R}, \mathrm{d}\nu)$ such that $U\psi = \mathbf{1}$ is the constant function $\mathbf{1}(E) = 1$, and UHU^{-1} is the operator of multiplication by the variable $E \in \mathbb{R}$. All other forms of the spectral theorem for self-adjoint operators can be deduced from this basic one.

The spectrum $\mathrm{sp}(H)$ of H is equal to the support $\mathrm{supp}(\nu)$ of ν. Spectral types are associated to the Lebesgue-Radon-Nikodym decomposition

$$\nu = \nu_{\mathrm{ac}} + \nu_{\mathrm{sc}} + \nu_{\mathrm{pp}},$$

where ν_{ac} is the part of ν which is absolutely continuous w.r.t. Lebesgue's measure, ν_{sc} is the singular continuous part, and ν_{pp} is the pure point (atomic) part,

$$\nu_{\mathrm{pp}}(S) = \sum_{E \in S} \nu(\{E\}).$$

The supports of these measures are respectively the absolutely continuous, singular continuous, and pure point spectrum of H,

$$\mathrm{sp}_a(H) = \mathrm{supp}(\nu_a), \qquad a \in \{\mathrm{ac}, \mathrm{sc}, \mathrm{pp}\}.$$

Obviously, $\mathrm{sp}(H) = \mathrm{sp}_{\mathrm{ac}}(H) \cup \mathrm{sp}_{\mathrm{sc}}(H) \cup \mathrm{sp}_{\mathrm{pp}}(H)$. The continuous part of the spectral measure is defined by $\nu_{\mathrm{cont}} = \nu_{\mathrm{ac}} + \nu_{\mathrm{sc}}$ and the singular part by $\nu_{\mathrm{sing}} = \nu_{\mathrm{sc}} + \nu_{\mathrm{pp}}$. The continuous and singular spectrum of H are respectively $\mathrm{sp}_{\mathrm{cont}}(H) = \mathrm{sp}_{\mathrm{ac}}(H) \cup \mathrm{sp}_{\mathrm{sc}}(H)$ and $\mathrm{sp}_{\mathrm{sing}}(H) = \mathrm{sp}_{\mathrm{sc}}(H) \cup \mathrm{sp}_{\mathrm{pp}}(H)$. The spectral subspaces associated to the spectral types are

$$\mathcal{H}_a = U^{-1}[L^2(\mathbb{R}, \mathrm{d}\nu_a)], \qquad a \in \{\mathrm{ac}, \mathrm{sc}, \mathrm{pp}, \mathrm{cont}, \mathrm{sing}\}.$$

Obviously, $\mathcal{H} = \mathcal{H}_{\mathrm{ac}} \oplus \mathcal{H}_{\mathrm{sc}} \oplus \mathcal{H}_{\mathrm{pp}} = \mathcal{H}_{\mathrm{cont}} \oplus \mathcal{H}_{\mathrm{pp}} = \mathcal{H}_{\mathrm{ac}} \oplus \mathcal{H}_{\mathrm{sing}}$. We set $U_a = U \restriction \mathcal{H}_a$ and denote by $\mathbb{1}_a$ the orthogonal projection onto $\mathcal{H}_a$. For any $\phi \in \mathcal{H}$,

$$(U_{\mathrm{ac}} \mathbb{1}_{\mathrm{ac}} \phi)(E) = \lim_{\varepsilon \downarrow 0} \frac{\langle \psi, [\mathrm{Im}\,(H - E - \mathrm{i}\varepsilon)^{-1}]\phi \rangle}{\mathrm{Im}\,\langle \psi, (H - E - \mathrm{i}\varepsilon)^{-1}\psi \rangle}, \qquad \text{for } \nu_{\mathrm{ac}} - \text{a.e. } E,$$

$$(U_{\mathrm{sing}} \mathbb{1}_{\mathrm{sing}} \phi)(E) = \lim_{\varepsilon \downarrow 0} \frac{\langle \psi, (H - E - \mathrm{i}\varepsilon)^{-1}\phi \rangle}{\langle \psi, (H - E - \mathrm{i}\varepsilon)^{-1}\psi \rangle}, \qquad \text{for } \nu_{\mathrm{sing}} - \text{a.e. } E.$$

One easily shows that

$$\frac{1}{\pi} \mathrm{Im}\, F(E + \mathrm{i}\varepsilon)\mathrm{d}E \to \mathrm{d}\nu(E)$$

weakly as $\varepsilon \downarrow 0$. Moreover:

i) For Lebesgue a.e. $E \in \mathbb{R}$ the limit $F(E + \mathrm{i}0) := \lim_{\varepsilon \downarrow 0} F(E + \mathrm{i}\varepsilon)$ exists, is finite, and

$$\mathrm{d}\nu_{\mathrm{ac}}(E) = \frac{1}{\pi} \mathrm{Im}\, F(E + \mathrm{i}0)\mathrm{d}E.$$

The set [4]

$$\Sigma_{\mathrm{ac}}(H) = \{E \,|\, \mathrm{Im}\, F(E + \mathrm{i}0) > 0\}$$

is the essential support of the absolutely continuous spectrum of H and $\mathrm{sp}_{\mathrm{ac}}(H)$ is the essential closure of $\Sigma_{\mathrm{ac}}(H)$.

ii) The measure ν_{sing} is concentrated on the set

$$\{E \,|\, \lim_{\varepsilon \downarrow 0} \mathrm{Im}\, F(E + \mathrm{i}\varepsilon) = \infty\}.$$

iii) Since for all $E \in \mathbb{R}$, $\nu(\{E\}) = \lim_{\varepsilon \downarrow 0} \varepsilon \mathrm{Im}\, F(E + \mathrm{i}\varepsilon)$, the set of eigenvalues of H is

$$\mathcal{E} := \{E \,|\, \lim_{\varepsilon \downarrow 0} \varepsilon \mathrm{Im}\, F(E + \mathrm{i}\varepsilon) > 0\}.$$

For $E \in \mathcal{E}$,

$$(U_{\mathrm{pp}} \mathbb{1}_{\mathrm{pp}} \phi)(E) = \lim_{\varepsilon \downarrow 0} \frac{\langle \psi, (H - E - \mathrm{i}\varepsilon)^{-1}\phi \rangle}{\langle \psi, (H - E - \mathrm{i}\varepsilon)^{-1}\psi \rangle}.$$

Obviously, $\mathrm{sp}_{\mathrm{pp}}(H)$ is the closure of $\mathcal{E}$.

[4] This set is defined modulo sets of Lebesgue measure zero.

The quantum mechanical interpretation of the triple $(\mathcal{H}, H, \psi)$ is that the wave function ψ describes a state and the operator H an observable of the quantum system under consideration. The result of a measurement of H is a random variable with values in $\mathrm{sp}(H)$ and with probability distribution ν. In what follows we shall restrict ourselves to the case where the observable H is the Hamiltonian of the system and $\mathrm{sp}(H)$ describes its possible energies. The Hamiltonian is also the generator of the dynamics, and the state of the system at time t is

$$\psi(t) = \mathrm{e}^{-\mathrm{i}tH}\psi.$$

If $\phi \in \mathcal{H}$ is a unit vector, then

$$p_\phi(t) = |\langle \phi, \mathrm{e}^{-\mathrm{i}tH}\psi\rangle|^2 = \left| \int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}tE}(U\phi)(E)\mathrm{d}\nu(E)\right|^2$$

is the probability that, at time t, the quantum mechanical system is in the state described by the wave function ϕ. It is a result of Kato that the absolutely continuous spectral subspace $\mathcal{H}_{\mathrm{ac}}$ is the closure of the linear span of ϕ's satisfying

$$\int_{\mathbb{R}} p_\phi(t)\mathrm{d}t < \infty.$$

It follows from Wiener's theorem that $\phi \in \mathcal{H}_{\mathrm{cont}}$ iff

$$\lim_{t\to\infty} \frac{1}{2t}\int_{-t}^{t} p_\phi(s)\mathrm{d}s = 0.$$

Finally, $\phi \in \mathcal{H}_{\mathrm{pp}}$ iff the function $t \mapsto p_\phi(t)$ is quasi-periodic.

The classical results described above lead to the following conclusions. The resolvent $(H-z)^{-1}$ and the Borel transform of ν identify the energies and subspaces of the spectral types. The spectral subspaces can be also characterized by $\mathrm{e}^{-\mathrm{i}tH}$ and the Fourier transform of ν. The basic intuition that the energies in $\mathrm{sp}_{\mathrm{ac}}(H)$ and the states in $\mathcal{H}_{\mathrm{ac}}(H)$ are linked to transport phenomena in the quantum system described by the triple $(\mathcal{H}, H, \psi)$ is partly captured in these characterizations. There is an enormous body of literature concerning refinement of the above rough picture. Detailed studies of the links between dynamics, transport, and spectrum reveal an intricate complex dependence that is only partly understood, and many basic questions remain open.

3 Jacobi matrix representation

Since $\dim \mathcal{H} = \infty$ the functions E^n, $n \geq 0$, are linearly independent in $L^2(\mathbb{R}, \mathrm{d}\nu)$. Since ν has bounded support, it follows from the Weierstrass theorem that these functions also span $L^2(\mathbb{R}, \mathrm{d}\nu)$. The Gram-Schmidt orthogonalization process thus yields an orthogonal basis of polynomials $\{P_n\}_{n\geq 0}$, where P_n has degree n and leading coefficient 1. Setting $p_n = P_n/\|P_n\|$, it follows that $\{p_n\}_{n\geq 0}$ is an orthonormal basis of $L^2(\mathbb{R}, \mathrm{d}\nu)$. For $n \geq 0$ set

$$a_{n+1} = \frac{\|P_{n+1}\|}{\|P_n\|}, \qquad b_{n+1} = \frac{1}{\|P_n\|^2}\int_{\mathbb{R}} E[P_n(E)]^2\mathrm{d}\nu(E).$$

With $p_{-1} \equiv 0$, the following basic relation holds:

$$E p_n(E) = a_{n+1} p_{n+1}(E) + b_{n+1} p_n(E) + a_n p_{n-1}(E). \tag{3.1}$$

In the orthonormal basis $\{p_n\}_{n\geq 0}$, the operator of multiplication by the variable $E \in \mathbb{R}$ on the Hilbert space $L^2(\mathbb{R}, \mathrm{d}\nu)$ is thus described by the Jacobi matrix

$$J = \begin{pmatrix} b_1 & a_1 & 0 & \\ a_1 & b_2 & a_2 & \ddots \\ 0 & a_2 & b_3 & \ddots \\ & \ddots & \ddots & \ddots \end{pmatrix}. \tag{3.2}$$

The matrix (3.2) defines a bounded self-adjoint operator on $\ell^2(\mathbb{N})$. The unitary map

$$\mathcal{U} : L^2(\mathbb{R}, \mathrm{d}\nu) \to \ell^2(\mathbb{N}), \qquad \mathcal{U} p_n = \delta_{n+1},$$

identifies the triples $(L^2(\mathbb{R}, \mathrm{d}\nu), E, \mathbf{1})$ and $(\ell^2(\mathbb{N}), J, \delta_1)$. Obviously, ν is the spectral measure for J and δ_1. Combined with the spectral theorem, this gives the identification between the spectral triples $(\mathcal{H}, H, \psi)$ and $(\ell^2(\mathbb{N}), J, \delta_1)$ mentioned in the introduction. Note in particular that H and J have the same spectral types.

Fixing E, $u_E(n) := p_{n-1}(E)$, $n \geq 1$, defines a sequence of real numbers. Relation (3.1) shows that this sequence is the unique solution of the Schrödinger equation $J u_E = E u_E$ with boundary conditions $u_E(0) = 0$, $u_E(1) = 1$. The generalized eigenfunctions $(u_E(n))_{n\geq 0}$ shed a different light on the spectral theory. E is an eigenvalue of J iff $\sum_n |u_E(n)|^2 < \infty$. As $n \to \infty$,

$$\frac{1}{\pi} \frac{1}{|u_E(n)|^2 + a_n^2 |u_E(n+1)|^2} \mathrm{d}E \to \mathrm{d}\nu(E)$$

weakly, see [Si4]. Furthermore, the generalized eigenfunctions are linked to the resolvent and the spectral types by

$$u_E(n) = \lim_{\varepsilon \downarrow 0} \frac{\operatorname{Im} \langle \delta_1, (J - E - \mathrm{i}\varepsilon)^{-1} \delta_n \rangle}{\operatorname{Im} \langle \delta_1, (J - E - \mathrm{i}\varepsilon)^{-1} \delta_1 \rangle} \qquad \text{for } \nu_{\mathrm{ac}} - \text{a.e. } E,$$

$$u_E(n) = \lim_{\varepsilon \downarrow 0} \frac{\langle \delta_1, (J - E - \mathrm{i}\varepsilon)^{-1} \delta_n \rangle}{\langle \delta_1, (J - E - \mathrm{i}\varepsilon)^{-1} \delta_1 \rangle} \qquad \text{for } \nu_{\mathrm{sing}} - \text{a.e. } E.$$

The following well-known bound holds:[5] for any $\epsilon > 0$ and for ν–a.e. E there is a finite constant $C_{E,\epsilon} > 0$ such that for all $n \geq 1$, $|u_E(n)| \leq C_{E,\epsilon} n^{1/2+\epsilon}$.

For a pedagogical exposition of the results presented in this section we refer the reader to [Si1].

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

4 Schrödinger Conjectures

The Schrödinger Conjectures concern deep refinements of the bound mentioned at the end of the previous section. 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 mathematics literature, such as the Steklov Conjecture [Ra, St]. The entire subject has a fascinating history which has been partly reviewed in [MMG].

The Schrödinger Conjecture for the pure point spectrum is trivial. For the singular continuous spectrum, it asserts that for all Jacobi matrices J, $\sup_{n\geq 1}|u_E(n)|<\infty$ for $\nu_{\rm sing}$-a.e. E. A counterexample to this conjecture was obtained by Jitomirskaya [Ji]. 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 $\nu_{\rm ac}$-a.e. E. In terms of the transfer matrices[6]

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

and using the invariance of ac spectrum under rank one perturbations[7], one arrives at the equivalent formulation

Schrödinger Conjecture I. For all Jacobi matrices J and $E\in\Sigma_{\rm ac}(J)$[8],

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

Among other partial results towards this conjecture, Gilbert and Pearson [GP] (see also [Si2]) showed that

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

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

$$\Sigma_{\rm ac}(J)\subset\{E\mid \liminf_{n\to\infty}\|T_E(n)\|<\infty\}. \tag{4.1}$$

Last and Simon [LS] refined the last result and established the following averaged form of Conjecture I:

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

[6]The convention on the $A_E(x)$ is such that their determinant is 1. Then u_E is a solution of the eigenvalue equation iff $\begin{bmatrix}u_E(n+1)\\ a_nu_E(n)\end{bmatrix}=A_E(n)\begin{bmatrix}u_E(n)\\ a_{n-1}u_E(n-1)\end{bmatrix}$.

[7]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, $\Sigma_{\rm ac}(J_\theta)=\Sigma_{\rm ac}(J)$ 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 $\begin{bmatrix}u_{E,\theta}(n+1)\\ a_nu_{E,\theta}(n)\end{bmatrix}=T_E(n)\begin{bmatrix}1\\ \theta\end{bmatrix}$, and ${\rm sp}_{\rm ac}(J)=\emptyset$ if $\liminf a_n=0$, the Schrödinger Conjecture for two different θ's gives $\sup_{n\geq 1}\|T_E(n)\|<\infty$.

[8]Recall that $\Sigma_{\rm ac}(J)$ denotes the essential support of the ac spectrum of J.

A particularly striking aspect of Avila's counterexample [Av] to the Schrödinger Conjecture I is that it concerns a spectrally rigid[9] class of Jacobi matrices describing discrete ergodic Schrödinger operators. In this setting $a_n = 1$ for all n 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. Ergodicity implies that there are deterministic sets $\Sigma_{\rm ac}$ and $\mathcal{B}$ such that for a.e. $\omega \in \Omega$, $\Sigma_{\rm ac} = \Sigma_{\rm ac}(J_\omega)$, $\mathcal{B} = \{E \mid \sup_{n\geq 1} \|T_E(\omega, n)\| < \infty\}$. Avila constructs Ω, B, and a uniquely 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 ACET Conjecture, discussed in Section 6:

Schrödinger Conjecture II. For all Jacobi matrices J,

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

Kotani's theory [Si3] gives that Conjecture II holds for Jacobi matrices describing 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 [BJLP2]:

Theorem 4.1 *For any Jacobi matrix J, any interval $]a, b[$, and any sequence $L_n \to \infty$ 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 7.

5 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 $\mathcal{H}_L = \ell^2(Z_L)$, $Z_L = \{1, \ldots, L\}$, and the one-particle Hamiltonian J_L, the restriction of J to Z_L with Dirichlet boundary conditions. The left/right electronic reservoir $\mathcal{R}_{l/r}$ is described by the spectral triple $(\mathcal{H}_{l/r}, H_{l/r}, \psi_{l/r})$. 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

[9] The rigidity here refers to Kotani theory [Si3].

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

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

where $\mathbb{1}_r$ is the orthogonal projection from $\mathcal{H}$ onto $\mathcal{H}_r$. We assume that the left/right 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 the 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 across the sample from the right to the left reservoir 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[10], one proves [AJPP, N]

$$\langle \mathcal{J}_L\rangle_+ := \lim_{t\to\infty}\frac{1}{t}\int_0^t \langle \mathcal{J}_L\rangle_s \mathrm{d}s = \frac{1}{2\pi}\int_{\mu_l}^{\mu_r}\mathcal{D}(L,E)\mathrm{d}E \tag{5.1}$$

where

$$\mathcal{D}(L,E) = 4\pi^2\lambda^4|\langle\delta_1,(H_\lambda - E - \mathrm{i}0)^{-1}\delta_L\rangle|^2\frac{\mathrm{d}\nu_{l,\mathrm{ac}}}{\mathrm{d}E}(E)\frac{\mathrm{d}\nu_{r,\mathrm{ac}}}{\mathrm{d}E}(E) \tag{5.2}$$

is the one-particle transmittance ($\nu_{l/r}$ being the spectral measure of $H_{l/r}$ for $\psi_{l/r}$). Relations (5.1) and (5.2) constitute the Landauer-Büttiker formula in the setting of our EBB model. We emphasize that its derivation is based on the first principles of quantum mechanics.

Note that $\Sigma_{l/r,\mathrm{ac}} := \{E\,|\,\frac{\mathrm{d}\nu_{l/r,\mathrm{ac}}}{\mathrm{d}E}(E) > 0\}$ 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 $\Sigma_{\mathrm{ac}}(J) \subset \Sigma_{l,\mathrm{ac}} \cap \Sigma_{r,\mathrm{ac}}$.

6 Linear response and Schrödinger Conjectures

Setting $\mu_l = \mu$, $\mu_r = \mu + \epsilon$, the Landauer-Büttiker formula gives[11]

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

The starting point of our research 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 [BJP], prior to Avila's announcement of the results [Av]:

[10] This assumption is harmless and can always be achieved by choosing appropriate reservoirs.

[11] In general, this relation holds for Lebesgue a.e. μ. However, one can always choose regular enough reservoirs so that it holds for all μ.

ACET Conjecture. For all Jacobi matrices J,

$$\underline{\mathcal{T}} = \overline{\mathcal{T}} = \Sigma_{\rm ac}(J).$$

The main result of [BJP] 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 give that the ACET Conjecture is equivalent to the Schrödinger Conjectures I + II. Avila's counterexample disproves $\underline{\mathcal{T}} = \Sigma_{\rm ac}(J)$, while the validity of $\overline{\mathcal{T}} = \Sigma_{\rm ac}(J)$ for all Jacobi matrices remains an open problem.

7 Characterization of the absolutely continuous spectrum

7.1 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, [BJLP2] shows that the large L asymptotics of the steady state current[12] fully characterizes the absolutely continuous spectrum.

Theorem 7.1 *For any Jacobi matrix J, any $\mu_r > \mu_l$, all reservoirs satisfying $]\mu_l, \mu_r[\subset \Sigma_{l,\rm ac} \cap \Sigma_{r,\rm ac}$, and any sequence of integers $L_n \to \infty$, one has*

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

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 4.1.

Theorem 7.1 extends to other notions of electronic transport common in the physics literature and we proceed to describe these results.

7.2 Thouless transport

The Thouless formula is a special case of the Landauer-Büttiker formula in which the reservoirs are implemented in such a way that the coupled Hamiltonian H_λ is a periodic Jacobi matrix; see Figure 2. More precisely, let $J_{L,\rm per}$ be the periodic Jacobi matrix on $\ell^2(\mathbb{Z})$ obtained by extending the Jacobi parameters $(a_n)_{1\leq n<L}$ and $(b_n)_{1\leq n\leq L}$ 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

[12] The associated conductances $G_L = \frac{1}{\mu_r - \mu_l}\langle \mathcal{J}_L\rangle_+$ play a similar role.

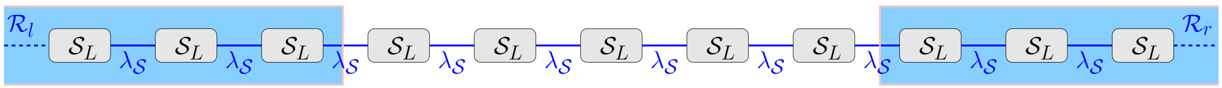

Figure 2: The periodic EBB model associated to the Hamiltonian $J_{L,\text{per}}$.

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 $J_{L,\text{per}}$ 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 $\lambda = \lambda_{\mathcal{S}}$. We shall refer to the corresponding EBB model as *crystalline*. For such EBB models the Landauer-Büttiker formula coincides with the Thouless formula[13]:

$$\langle \mathcal{J}_L^{\text{Th}}\rangle_+ = \frac{1}{2\pi}\,|\text{sp}(J_{L,\text{per}})\cap]\mu_l,\mu_r[\,|\,, \tag{7.1}$$

where $|\cdot|$ denotes Lebesgue measure. For Thouless transport we also have [BJLP2]:

Theorem 7.2 *For any Jacobi matrix J, any $\mu_r > \mu_l$ and any sequence of integers $L_n \to \infty$ one has*

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

The proof again proceeds by showing that $\lim\langle\mathcal{J}_{L_n}^{\text{Th}}\rangle_+ = 0 \Leftrightarrow \lim\int_{\mu_l}^{\mu_r}\|T_E(L_n)\|^{-2}\text{d}E = 0$. The details of the proof, however, are considerably more involved than in the case of Theorem 7.1.

7.3 Crystalline transport

A third notion of electronic transport, called Crystalline transport, was introduced in [BJLP1] as a link between Landauer-Büttiker and Thouless transports. It arises by considering an approximation of $J_{L,\text{per}}$ by finite repetitions of the sample connected to arbitrary reservoirs.

More precisely, let $J_{L,\text{per}}$ be as in the previous section. Given a positive integer N, let $J_L^{(N)}$ be the restriction of $J_{L,\text{per}}$ to $Z_{NL} = \{1,\ldots,NL\}$ with Dirichlet boundary condition, i.e. $J_L^{(N)}$ is a Jacobi matrix acting on $\ell^2(Z_{NL})$ whose Jacobi parameters satisfy

$$a_{x+nL} = a_x, \qquad bx + nL = b_x, \qquad n = 0,1,\ldots,N-1,\ x\in Z_L,$$

where $\{a_x\}_{1\le x<L}$ and $\{b_x\}_{1\le x\le L}$ are the Jacobi parameters of the original sample Hamiltonian J_L and $a_L = \lambda_{\mathcal{S}}$ is the internal coupling constant. The pairs $(\ell^2(Z_{NL}), J_L^{(N)})$ define a sequence of sample systems coupled at their endpoints to the reservoirs $\mathcal{R}_{l/r}$ as in Section 5; see Figure 3. The reservoirs are described by spectral triples $(\mathcal{H}_{l/r}, H_{l/r}, \psi_{l/r})$. Neither the reservoirs nor the coupling strength λ depend on N. Denoting by $\langle\mathcal{J}_L^{(N)}\rangle_+$ the Landauer-Büttiker current in this EBB model, it is proven in [BJLP1] that

$$\langle\mathcal{J}_L^{\text{Cr}}\rangle_+ := \lim_{N\to\infty}\langle\mathcal{J}_L^{(N)}\rangle_+ = \int_{\text{sp}(J_{L,\text{per}})\cap]\mu_l,\mu_r[}\mathcal{D}_L^{\text{Cr}}(E)\text{d}E, \tag{7.2}$$

[13] We refer the reader to [BJLP1] for a detailed discussion regarding the identification of (7.1) with the usual heuristically derived Thouless conductance formula found in the physics literature.

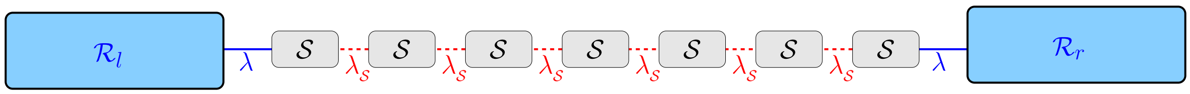

Figure 3: The EBB model associated to the sample hamiltonian $J_L^{(N)}$ for $N = 7$.

where

$$\mathcal{D}_L^{\rm Cr}(E) := \left[1 + \frac{1}{4}\left(\frac{|\lambda_{\mathcal{S}}^2 m_r(E) - \lambda^2 F_r(E)|^2}{{\rm Im}\,(\lambda_{\mathcal{S}}^2 m_r(E)){\rm Im}\,(\lambda^2 F_r(E))} + \frac{|\lambda_{\mathcal{S}}^2 m_l(E) - \lambda^2 F_l(E)|^2}{{\rm Im}\,(\lambda_{\mathcal{S}}^2 m_l(E)){\rm Im}\,(\lambda^2 F_l(E))}\right)\right]^{-1} \tag{7.3}$$

for $E \in {\rm sp}(J_{L,{\rm per}}) \cap \Sigma_{l,{\rm ac}} \cap \Sigma_{r,{\rm ac}}$.[14] In this formula $F_{l/r}(E) := \langle \psi_{l/r}, (H_{l/r} - E - {\rm i}0)^{-1}\psi_{l/r}\rangle$,

$$m_l(E) = \langle \delta_0, (J_{L,{\rm per}}^{(l)} - E - {\rm i}0)^{-1}\delta_0\rangle, \qquad \text{and} \qquad m_r(E) = \langle \delta_1, (J_{L,{\rm per}}^{(r)} - E - {\rm i}0)^{-1}\delta_1\rangle,$$

where $J_{L,{\rm per}}^{(l)}/J_{L,{\rm per}}^{(r)}$ is the restriction of $J_{L,{\rm per}}$ to $\ell^2((-\infty, 0]\cap\mathbb{Z})/\ell^2([1,\infty)\cap\mathbb{Z})$ with Dirichlet boundary condition.

The formulas (7.2) and (7.3) give

$$\langle \mathcal{J}_L^{\rm Th}\rangle_+ = \sup\ \langle \mathcal{J}_L^{\rm Cr}\rangle_+, \tag{7.4}$$

where the supremum is taken over all realizations of the reservoirs. The supremum is achieved iff the EBB model is crystalline; see Section 7.2. We refer the reader to [BJLP1] for more details. Eq. (7.4) is a mathematically rigorous justification of the well-known heuristic statement that the Thouless transport is the maximal transport at zero temperature for the given chemical potential interval $]\mu_l, \mu_r[$. The fact that the above supremum is achieved iff the EBB model is crystalline also identifies the heuristic notion of "optimal feeding" of electrons with reflectionless transport between the reservoirs.

Our final result states that crystalline transport also fully characterizes the absolutely continuous spectrum [BJLP3]:

Theorem 7.3 *For any Jacobi matrix J, any $\mu_r > \mu_l$, all reservoirs satisfying $]\mu_l, \mu_r[\subset \Sigma_{l,{\rm ac}} \cap \Sigma_{r,{\rm ac}}$, and any sequence of integers $L_n \to \infty$, one has*

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

The proof proceeds by showing that $\lim_{n\to\infty}\langle \mathcal{J}_{L_n}^{\rm Cr}\rangle_+ = 0 \Leftrightarrow \lim_{n\to\infty}\langle \mathcal{J}_{L_n}^{\rm Th}\rangle_+ = 0$ (one direction is immediate using (7.4)) and by invoking Theorem 7.2.

8 Concluding remarks

The main novelty of the research program developed in [BJP, BJLP1, BJLP2, BJLP3] concerns the identification of an appropriate notion of transport for a spectral triple $(\mathcal{H}, H, \psi)$ and in relating this transport to the ac spectrum. The main steps are:

[14] Outside this set, one sets $\mathcal{D}_L^{\rm Cr}(E) = 0$.

1. Associate to $(\mathcal{H}, H, \psi)$, via a canonical procedure, a unitarily equivalent spectral triple of the form $(\ell^2(\mathbb{N}), J, \delta_1)$ where J is a Jacobi matrix.

2. Consider the sequence of EBB models, indexed by $L \in \mathbb{N}$, in which two electronic reservoirs, at zero temperature and chemical potential μ_l/μ_r, are attached at the end points of the finite sample obtained by restricting J to the interval $\{1, \ldots, L\}$. The voltage differential $\mu_r - \mu_l$ then generates an electronic current through the sample with the steady state value $\langle \mathcal{J}_L \rangle_+$.

3. Link the ac spectrum of $(\mathcal{H}, H, \psi)$ to the large L behavior of $\langle \mathcal{J}_L \rangle_+$.

The results presented in this note, Theorems 7.1, 7.2 and 7.3, identify the ac spectrum with the set of energies for which the current $\langle \mathcal{J}_L \rangle_+$ persists as L goes to infinity. More colloquially, they establish the equivalence between the mathematical and the physical characterization of the conducting regime.

These results also naturally lead to questions regarding the relative scaling, and the rate of convergence to zero, of the various steady currents $\langle \mathcal{J}_L \rangle_+$, $\langle \mathcal{J}_L^{\mathrm{Th}} \rangle_+$ and $\langle \mathcal{J}_L^{\mathrm{Cr}} \rangle_+$ in the regime $\mathrm{sp}_{\mathrm{ac}}(H) \cap]\mu_l, \mu_r[= \emptyset$. Although these questions played a prominent role in early physicists works on the subject (see, e.g., [AL, CGM]), we are not aware of any mathematically rigorous works on this topic. We plan to address these problems in the continuation of our research program.

The above scheme also opens a new way to approach the fundamental and mostly open question of many-body localization. One adds to the "independent electron" Hamiltonian $\mathrm{d}\Gamma(H_\lambda)$ of the combined sample-reservoirs system, see Section 5, an interaction term of the form

$$W := \frac{\kappa}{2} \sum_{m,n \in Z_L,} v(|m-n|) a^*(\delta_m) a^*(\delta_n) a(\delta_n) a(\delta_m), \qquad \kappa \in \mathbb{R},$$

where v is a short range pair potential. The interaction term does not change the electronic current observable,

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

and we set

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

where ω_{μ_l,μ_r} is as in Section 5. Finally, let[15]

$$\langle \mathcal{J}_L \rangle_{+,\mathrm{inf}} := \liminf_{t\to\infty} \frac{1}{t} \int_0^t \langle \mathcal{J}_L \rangle_s \mathrm{d}s, \qquad \langle \mathcal{J}_L \rangle_{+,\mathrm{sup}} := \limsup_{t\to\infty} \frac{1}{t} \int_0^t \langle \mathcal{J}_L \rangle_s \mathrm{d}s.$$

We say that

- $]\mu_l, \mu_r[$ is in the localization regime if $\limsup_{L\to\infty} \langle \mathcal{J}_L \rangle_{+,\mathrm{sup}} = 0$;
- $]\mu_l, \mu_r[$ is in the conducting regime if $\liminf_{L\to\infty} \langle \mathcal{J}_L \rangle_{+,\mathrm{inf}} > 0$;

[15] It is known that if the reservoirs are sufficently regular, then $\langle \mathcal{J}_L \rangle_{+,\mathrm{inf}} = \langle \mathcal{J}_L \rangle_{+,\mathrm{sup}}$ for $|\kappa| < \kappa_L$, where $\kappa_L \to 0$ as $L \to \infty$; see [JOP]. The validity of this relation for all L and κ is an open problem.

When $\kappa = 0$, Theorem 7.1 gives that these definitions are equivalent to the absence/presence of the ac spectrum in the interval $]\mu_l, \mu_r[$. The proposed dynamical definition of the localization/conduction regime for an interacting $1d$ lattice electron gas appears to be new and allows for a mathematically precise formulation of a number of problems related to many-body localization. This topic remains to be studied in the future.

Finally, since our approach and results apply to any (abstract) spectral triple irrespectively of its physical origin, they can be also viewed as a part of the general structural link between spectral theory and quantum mechanics.

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