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Subdiffusive Quantum Transport for 3D Hamiltonians with Absolutely Continuous Spectra

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We exhibit a class of Hamiltonians in dimension $D \geqslant 3$, describing a quantum particle in an aperiodic medium with absolutely continuous spectrum and subdiffusive behavior. The diffusion exponent, which characterizes the time growth of the mean square displacement, can be chosen slightly bigger than Guarneri's lower bound. These models are built out of 1D Hamiltonians with well-understood spectral and transport properties.

KEY WORDS: Anomalous quantum transport; fractal measures.

Quantum diffusion in aperiodic media is slowed down due to destructive interference phenomena. The most prominent example is the Anderson model describing an electron in a disordered potential. In low dimension or for a strong disordered potential, the motion is completely localized and the spectrum is known to be pure-point (see 1 and references therein). On the other hand, scaling arguments and numerical calculations[(18)] show that, in three dimensions and at low disorder, the motion is diffusive while the spectrum is expected to be absolutely continuous. 3D quasicrystals are other interesting systems in which the spectral measures are probably absolutely continuous whereas numerics show that the quantum transport is even subdiffusive.[(25)] This subdiffusive motion plays a crucial role in qualitative explanations of the experimental results on electronic transport in quasicrystals.[(29, 19, 26)]

The purpose of this note is to exhibit an aperiodic tight-binding Hamiltonian in dimension $D \geqslant 3$ with absolutely continuous spectrum, but

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subdiffusive quantum transport. It is constructed as a linear combination of 1D tight-binding Hamiltonians Hj, $j=1...D$, acting on $\ell^2(\Lambda)$ where $\Lambda=\mathbf{Z}$ or $\Lambda=\mathbf{N}$, as follows:

$$H^\eta=\sum_{j=1}^{D}\eta_j \mathbf{1}\otimes\cdots\otimes H_j\otimes\cdots\otimes\mathbf{1}:\ell^2(\Lambda^{\times D})\to\ell^2(\Lambda^{\times D}) \tag{1}$$

Here $\eta=(\eta_1,..., \eta_D)\in\mathbf{R}_+^D$. This simple construction is well-known. It is similar to the labyrinth model introduced by Sire.[28] Recently it has also been used by Simon.[27]

The 1D models H_j will be chosen as Jacobi matrices with self-similar fractal spectra[5, 6, 9, 20, 10] for which the transport properties have recently been analyzed rigorously.[10, 2] For the special case of certain limit-periodic Julia matrices[5, 4, 6] defined below, we will show that for $D=3$ and almost every η, the local density of states, namely the spectral measure of H^η, is absolutely continuous while the quantum motion is subdiffusive with a diffusion exponent only slightly larger than imposed by Guarneri's lower bound.

These examples may look artificial. They certainly differ from real quasicrystals. Nevertheless they constitute the first examples of homogenous finite-dimensional Hamiltonians for which spectral and anomalous transport properties can be controlled rigorously. A class of infinite-dimensional Hamiltonians with absolutely continuous spectral measure and diffusion exponents varying from 1 to 0 was previously constructed by Vidal, Mosseri and Bellissard.[30] We further acknowledge that Last and Kiselev recently studied another 3D Hamiltonian with absolutely continuous spectrum and subdiffusive quantum transport.[17]

We first define the diffusion exponents of a Hamiltonian H acting on a D-dimensional tightbinding Hilbert space $\ell^2(\Lambda^{\times D})$. Let $A(t)$ denote the time evolution of a given observable A and let $\vec{X}$ be the position operators on $\ell^2(\Lambda^{\times D})$. For $\alpha>0$ and $\psi\in\ell^2(\Lambda^{\times D})$ a state with compact support, we set

$$\beta_\alpha^\pm(H,\psi)=\lim_{T\to\infty}{}^{\pm}\frac{\log(\int_0^T\langle\psi|\,|\vec{X}|^\alpha(t)\,|\psi\rangle\,dt/T)}{\log(T^\alpha)} \tag{2}$$

where $\lim^+$ and $\lim^-$ denote the superior and inferior limit respectively. Note that an intermediate exponent between β^- and β^+ has also been defined by using Mellin's transform.[26] By functional calculus $|\vec{X}(t)|^\alpha=|\vec{X}|^\alpha(t)$. Elementary inequalities further show that $|\vec{X}(t)|^\alpha$ in (2) can be replaced by $|\vec{X}(t)-\vec{X}|^\alpha$ without changing the diffusion exponents. The (disorder or phase-averaged) diffusion exponent β_2 is of particular physical importance because it characterizes the low-temperature behavior of the direct conductivity as given by Kubo's formula in the relaxation time approximation.[26]

There are general relations between transport exponents and spectral properties of the Hamiltonian. It is usually accepted that, the smoother the spectral measures, the faster the wavepacket propagation, leading to large diffusion exponents. Guarneri[8] and others[7, 16, 11] proved a general inequality making this more quantitative:

$$\beta_\alpha^-(H, \psi) \geqslant \frac{1}{D}\dim_{\mathbf{H}}(\mu), \qquad \beta_\alpha^+(H, \psi) \geqslant \frac{1}{D}\dim_{\mathbf{P}}(\mu), \qquad \forall \alpha > 0$$

Here $\dim_{\mathbf{H}}(\mu)$ and $\dim_{\mathbf{P}}(\mu)$ are respectively the Hausdorff and packing dimension of the spectral measure μ of H with respect to ψ defined to be the μ-essential supremum of respectively the lower and upper pointwise dimensions $d_\mu^\pm(E) = \lim_{\varepsilon \to 0}^\pm \log(\mu([E-\varepsilon, E+\varepsilon]))/\log(\varepsilon)$. Both the Hausdorff and the packing dimension of μ only depend on the measure class of μ.[26, 12] For an absolutely continuous measure μ, one has $\dim_{\mathbf{H}}(\mu) = \dim_{\mathbf{P}}(\mu) = 1$.[26] Hence in dimension $D = 1$, absolutely continuous spectrum implies ballistic transport ($\beta_\alpha = 1$), while in dimension $D = 3$, absolutely continuous spectrum and subdiffusive motion ($\beta_\alpha < 1/2$) may coexist. Here we construct an example for this.

This lower bound has recently been improved[12, 3] using multifractal dimensions defined by:

$$D_\mu^\pm(q) = \lim_{q \to q'} \frac{1}{q'-1} \lim_{\varepsilon \to 0}^\pm \frac{\log(\int d\mu(E)\, \mu([E-\varepsilon, E+\varepsilon])^{q'-1}}{\log(\varepsilon)}, \qquad q \in \mathbf{R} \tag{3}$$

Then one gets:

$$\beta_\alpha^\pm(H, \psi) \geqslant \frac{1}{D} D_\mu^\pm\left(\frac{D}{D+\alpha}\right), \qquad \forall \alpha > 0 \tag{4}$$

Note that in several recent papers[9, 12, 3] the fact that $\beta_\alpha^\pm(H, \psi)$ be increasing with α is called *intermittency*.

Let now ψ be a tensor product state of the form $\psi = \psi_1 \otimes \cdots \otimes \psi_D$. We observe that the diffusion exponents of a Hamiltonian H^η of the form (1) satisfy

$$\beta_\alpha^+(H^\eta, \psi) = \max_{j=1 \cdots D} \beta_\alpha^+(H_j, \psi_j) \tag{5}$$

This follows directly from (1), (2) and the following inequality

$$\frac{1}{c}\sum_{j=1}^{D} y_j^{\alpha} \leqslant \left(\sum_{j=1}^{D} y_j\right)^{\alpha} \leqslant c \sum_{j=1}^{D} y_j^{\alpha}$$

valid for any $y_j \geqslant 0$, $j = 1 \cdots D$, where c is a positive constant depending only on D and α.

Let further $\mu_j^{\eta_j}$ be the spectral measure of $\eta_j H_j$ relative to ψ_j where $\eta_j > 0$. We get $\mu_j^{\eta_j}(\Delta) = \mu_j(\Delta/\eta_j)$ for all Borel subsets Δ of $\mathbf{R}$ where μ_j is the spectral measure of H_j. Then the spectral measure μ of H^η relative to ψ is nothing but the convolution of the $\mu_j^{\eta_j}$'s. Due to the smoothening properties of the convolution, it is possible for H^η to have absolutely continuous spectrum even though each H_j has a singular one. This will be made more explicit below.

We will choose the H_j's among the 1D models already investigated rigorously in refs. 10 and 2. These models exhibit anomalous transport and have a singular continuous spectrum. Their construction by inverse theory as Jacobi matrices with self-similar fractal spectrum is as follows. Let I_0^1 and I_1^1 be two disjoint closed intervals contained in a closed interval I^0. Let S be a smooth real function such that its restrictions $S_{0,1} : I_{0,1}^1 \to I^0$ are bijective with smooth inverse and such that $S(I^0 \backslash (I_0^1 \cup I_1^1)) \cap I^0 = \emptyset$. The inverse images $S^{-N}(I^0)$ consist of 2^N intervals of generation N. A coding $\sigma = (\sigma_i)_{i \geqslant 1}$ with $\sigma_i \in \{0, 1\}$ permits to describe them through $I_\sigma^N = S_{\sigma_1}^{-1} \circ \cdots \circ S_{\sigma_N}^{-1}(I^0)$. Finally S is supposed to be expansive, namely we suppose that there exist positive constants $a < 1$ and b such that the lengths of I_σ^N decrease faster than ba^N uniformly in σ.

Let μ_0 be an S-invariant ergodic measure supported by $J \subset \mathbf{R}$ obtained as the pull back of a shift-invariant ergodic measure on the code space. Whenever μ_0 is a Gibbs measure, its generalized dimensions defined by Eq. (3) coincide $D_{\mu_0}^+(q) = D_{\mu_0}^-(q)$ and are analytic in q (see ref. 23 and references therein). Furthermore, the measure μ_0 is exactly scaling, namely the pointwise dimensions $d_{\mu_0}(E) = \lim_{\varepsilon \to 0} \log(\mu_0([E - \varepsilon, E + \varepsilon]))/\log(\varepsilon)$ exist μ_0-almost surely and are μ_0-almost surely equal to $\dim_{\mathbf{H}}(\mu_0) = \dim_{\mathbf{P}}(\mu_0) = D_{\mu_0}(1)$.[23, 10]

Let $(P_n)_{n \geqslant 0}$ be the family of real orthonormal polynomials relative to the Hilbert space $L^2(\mathbf{R}, \mu_0)$. They satisfy a three term recurrence relation:

$$E P_n(E) = t_{n+1} P_{n+1}(E) + v_n P_n(E) + t_n P_{n-1}(E),$$
$$\forall n \in \mathbf{N}, \quad P_{-1} = 0, \quad P_0 = 1$$

where $t_0 = 0$, $t_n > 0$ for $n \geqslant 1$ and $v_n \in \mathbf{R}$. Equivalently, they define a tridiagonal selfadjoint matrix H_0 acting on $\ell^2(\mathbf{N})$ by $\langle n | H_0 | n+1 \rangle = t_{n+1}$

and $\langle n| H_0 |n\rangle = v_n$. It is the Jacobi matrix with self-similar spectral measure μ_0. Hence, the position operator for such matrices is constructed entirely from the spectral measure. It is thus expected that the diffusion properties, in particular the diffusion exponents, can be derived entirely from spectral properties. Actually, in refs. 10 and 2 upper bounds on the diffusion exponents of H_0 were given in purely spectral terms whenever the restrictions $S_{0,1}$ are polynomials.

In this work, we first focus on the example of Julia matrices and will then briefly comment on other cases below. A real Julia set is generated by the mapping $S(E) = E^2 - \lambda$, $\lambda > 2$. It satisfies all the above hypothesis. As measure μ_0, we choose a balanced Bernoulli measure, notably we suppose the σ_j's to be independent identically distributed random variables equal to 0 or 1 with equal probabilities. The corresponding Jacobi matrix H_0, also called a Julia matrix, obeys an exact renormalization group equation leading to a recurrence relation for the t_n's and $v_n = 0$, so that the sequence $(t_n)_{n \geqslant 0}$ is limit-periodic.[5, 4, 6]

The results on quantum transport are the following. For a real Julia matrix H_0, Mantica[20] has derived and checked numerically the following relation (for $\psi_0 = |0\rangle$ the localized state at the origin):

$$\beta_\alpha^{\pm}(H_0, \psi_0) = D_{\mu_0}(1-\alpha), \qquad \alpha > 0 \tag{6}$$

In refs. 10 and 2 it has been proved rigorously that $\beta_\alpha^+(H_0, \psi_0) \leqslant D_{\mu_0}(1-\alpha)$ for $\alpha \in (0, \alpha_c(\lambda)]$ and some $\alpha_c(\lambda) > 2$. The general inequality (4) gives a lower bound $\beta_\alpha^+(H_0, \psi_0) \geqslant D_{\mu_0}(1/(1+\alpha))$. These inequalities can be directly transposed to any compactly supported ψ_0. Therefore, the transport exponents of Julia matrices are determined only by the spectral measure. In particular, the intermittency, namely the fact that $\alpha \mapsto \beta_\alpha^+(H_0)$ is an increasing curve, is due to the non-trivial thermodynamics of the spectral measure.

Using (1) we now construct higher dimensional models with the same transport properties. Their spectral properties are given through the following theorem, a corollary of results obtained in ref. 13:

Theorem. Let $\mu_1,..., \mu_D$ be exactly scaling Borel measures on $\mathbf{R}$ and $\eta_1,..., \eta_D \in \mathbf{R}_+$. Let $\mu_j^{\eta_j}$ be the measure defined by $\mu_j^{\eta_j}(\Delta) = \mu_j((1/\eta_j)\, \Delta)$ for all Borel sets $\Delta \subset \mathbf{R}$. Then their convolution product satisfies

$$\dim_{\mathrm{H}}(\mu_1^{\eta_1} * \cdots * \mu_D^{\eta_D}) = \min\left\{1, \sum_{j=1}^{D} \dim_{\mathrm{H}}(\mu_j)\right\} \tag{7}$$

for Lebesgue almost all $\eta_1,..., \eta_D$. Moreover, if $\sum_{j=1}^{D} \dim_{\mathrm{H}}(\mu_j) > 1$, then $\mu_1^{\eta_1} * \cdots * \mu_D^{\eta_D}$ is absolutely continuous for Lebesgue almost all $\eta_1,..., \eta_D$.

On the right hand side of (7), $\dim_{\mathrm{H}}(\mu_j)$ can be replaced by $\dim_{\mathrm{H}}(\mu_j^{\eta_j})$ because the mapping $E \mapsto E/\eta_j$ is bi-Lipschitz and therefore does not change the Hausdorff dimension and pointwise dimensions (that is, $d_{\mu_j^{\eta_j}}(\eta_j E) = d_{\mu_j}(E)$). The theorem cannot be true for all $\eta_1,..., \eta_D$ because of resonance phenomena: see ref. 14 for such an example. For the proof of the theorem, one notes that $\mu_1^{\eta_1} * \cdots * \mu_D^{\eta_D}$ is the image of the product measure $\mu_1 \otimes \cdots \otimes \mu_D$ under the one-dimensional projection $P_\eta\colon \mathbf{R}^D \to \mathbf{R}$ given by $P_\eta(E_1,..., E_D) = \sum_{j=1}^{D} \eta_j E_j$ where $\eta = (\eta_1,..., \eta_D)$. Now it is shown in ref. 13 that, first of all, the Hausdorff dimension of a sum of exactly scaling measures is given by the sum of the Hausdorff dimensions of the summands, and, second of all, that the Hausdorff dimension of the one-dimensional projection $P_\eta(\nu)$ of a measure ν on $\mathbf{R}^D$ is equal to $\min\{1, \dim_{\mathrm{H}}(\nu)\}$ for Lebesgue almost all directions η. Actually ref. 13 only contains proofs for the case $D = 2$, but these proofs can be directly transposed to the finite-dimensional case by using the results of ref. 22 generalizing those of ref. 21. The second statement of the theorem follows similarly from ref. 13.

Let us use this result to construct the desired examples. Let μ_0 be an exactly scaling measure on a self-similar fractal set J invariant under the map S. The dilated measure μ_0^η, $\eta \in \mathbf{R}_+$, is supported on the set ηJ which is invariant under the map S_η defined by $S_\eta(E) = \eta S(E/\eta)$. As dilations are bi-Lipschitz maps and thus leave Hausdorff dimensions invariant, it follows from multifractal analysis that $D_{\mu_0}(q) = D_{\mu_0^\eta}(q)$ for all $q \in \mathbf{R}$. Combining all the above, we therefore obtain the following:

Theorem. Let $\mu_1,..., \mu_D$ be balanced Bernoulli measures on real Julia sets and $H_1,..., H_D$ their Jacobi matrices. Set $\psi = |0\rangle \otimes \cdots \otimes |0\rangle$. Then the Hamiltonian H^η defined in (1) as well as its spectral measure μ^η with respect to ψ satisfy for Lebesgue almost all $\eta = (\eta_1,..., \eta_D) \in \mathbf{R}_+^D$ and all $\alpha > 0$:

(i) $\dim_{\mathrm{H}}(\mu^\eta) = \min\{1, \sum_{j=1}^{D} \dim_{\mathrm{H}}(\mu_j)\}$.

(ii) If $\sum_{j=1}^{D} \dim_{\mathrm{H}}(\mu_j) > 1$, then μ^η is absolutely continuous.

(iii) $\beta_\alpha^+(H^\eta, \psi) \leqslant \max_{j=1\cdots D} D_{\mu_j}(1-\alpha)$ and
$\beta_\alpha^-(H^\eta, \psi) \geqslant \max_{j=1\cdots D} D_{\mu_j}(1/(1+\alpha))$.

Let us consider the concrete example of a Julia set for which $\dim_{\mathrm{H}}(\mu) = D_\mu(1) \approx 1/3$. This happens for $\lambda \approx 16.5$. The corresponding value of $D_\mu(-1)$ is 0.3342 (these numbers are by courtesy of G. Mantica). Hence the theorem guarantees the existence of a 3D model with absolutely continuous local density of states for which the diffusion exponent $\beta_2(H)$ is only slightly bigger than imposed by Guarneri's lower bound $\beta_2(H) \geqslant 1/D = 1/3$ (Eq. (4) gives a slightly better lower bound). We further dispose of 3D models with absolutely continuous spectrum and a diffusion exponent taking an arbitrary value in the interval $[0.3342, 1]$.

Analogous results can be obtained for sums H^η of other models considered in refs. 10 and 2. Examples are Bernoulli measures on uniform Cantor sets generated by the mappings $S(E) = |\lambda E| - \lambda + 1$, $\lambda > 2$. The spectral properties of the corresponding H^η can be analyzed just as above, but the formulas for the upper bounds are more involved.[10] In absence of an exact renormalization property, the asymptotic properties of the generalized eigenfunctions certainly play an important role,[15, 20, 10] but a satisfactory theory does not seem available yet.

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