Subdiffusive quantum transport for $3D$-Hamiltonians with absolutely continuous spectra

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Abstract

Both in the $3D$ Anderson model at low disorder and in $3D$ quasicrystals, the local density of states is expected to be absolutely continuous, although the quantum transport is diffusive or subdiffusive respectively. By studying sums of $1D$ models with well-understood spectral and transport properties, we exhibit a $3D$ model with absolutely continuous spectrum for which the diffusion exponent characterizing the growth of the mean square displacement is only slightly bigger than imposed by Guarneri's lower bound.

Keywords: 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 [14] 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 [21]. This subdiffusive motion plays a crucial role in qualitative explanations of the experimental results on electronic transport in quasicrystals [25, 15, 22].

The purpose of this note is to exhibit an aperiodic tight-binding Hamiltonian in dimension $D \geq 3$ with absolutely continuous spectrum, but subdiffusive quantum transport. It is constructed as a linear combination of $1D$ tight-binding Hamiltonians H_j, $j = 1 \dots D$, acting on $\ell^2(\Lambda)$ where $\Lambda = \mathbf{Z}$ or $\Lambda = \mathbf{N}$:

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

Here $\eta = (\eta_1,\ldots,\eta_D) \in \mathbf{R}_+^D$. This simple construction is well-known in mathematical physics. It is similar to the labyrinth model introduced by Sire [24]. Recently it has also be used by Simon [23].

Our building kit of $1D$ models consists of Jacobi matrices with self-similar fractal spectra [4, 5, 7, 16, 8] for which the transport properties have recently been analized rigorously [8, 2]. For the special case of certain limit-periodic Julia matrices [4, 3, 5] 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.

Our examples are artificial and differ from real-life quasicrystals. Nevertheless they constitute the first examples of homogenous finite-dimensional Hamiltonians for which spectral and anomalous transport properties can be controled rigorously. An infinte-dimensional Hamiltonian with absolutely continuous spectral measure, but localized quantum motion was previously constructed by Vidal, Mosseri and Bellissard [26]. We further acknowledge that Last and Kiselev recently studied another $3D$ Hamiltonian with absolutely continuous spectrum and subdiffusive quantum transport [13].

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

$$\beta_\alpha^+(H,\psi) \;=\; \limsup_{T\to\infty} \frac{\log\left(\int_0^T \langle\psi|\,|\vec{X}|^\alpha(t)\,|\psi\rangle \; dt/T\right)}{\log(T^\alpha)} \;. \tag{2}$$

The diffusion exponent $\beta_\alpha^+(H)$ is then defined by taking the supremum over all compactly supported states ψ. A lower exponent $\beta_\alpha^-(H)$ can be introduced by replacing the limsup by liminf, an intermediate exponent by using the Mellin transform [22]. Note that $|\vec{X}(t)|^\alpha = |\vec{X}|^\alpha(t)$ by functional calculus. Some 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. Let us remark that the diffusion exponent $\beta_2(H)$ 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 [22].

The interesting issue is now to link the transport exponents to spectral properties of the Hamiltonian. The general wisdom states that continuity properties of the spectal measures lead to fast wavepacket propagation and hence large diffusion exponents. Guarneri [6] proved a general inequality making this quantitative:

$$\beta_\alpha^-(H) \;\geq\; \frac{1}{D}\,\dim_{\mathrm{H}}(\mu) \;, \qquad \forall\;\; \alpha > 0 \;.$$

Here $\dim_{\mathrm{H}}(\mu)$ is the Hausdorff dimension of the local density of states μ of H defined to be μ-essential supremum of the lower pointwise dimensions $d_\mu^-(E) = \liminf_{\epsilon\to 0}\log(\mu([E-\epsilon, E+\epsilon]))/\log(\epsilon)$. The Hausdorff dimension $\dim_{\mathrm{H}}(\mu)$ depends only on the measure class of μ [22]. For an absolutely continuous measure μ, one has $\dim_{\rm H}(\mu) = 1$ [22]. 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.

After these general discussions, let us next observe that the diffusion exponents of a Hamiltonian H^η of the form (1) satisfy

$$\beta_\alpha^+(H^\eta) \;=\; \max_{j=1\ldots D}\; \beta_\alpha^+(H_j)\;. \tag{3}$$

Actually, after having replaced (1) in (2), this follows directly from the inequality

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

holding for any $y_j \geq 0$, $j = 1\ldots D$, with a constant c depending only on D and α.

Now the spectral measure of H^η is the convolution of the dilated measured $\mu_j^{\eta_j}$ of the spectral measures μ_j of the H_j. It is defined by $\mu_j^{\eta_j}(\Delta) = \mu_j(\frac{1}{\eta_j}\Delta)$ for all Borel sets $\Delta \subset \mathbf{R}$. Due to the smoothening properties of the convolution, it is possible that H^η has absolutely continuous spectrum even though each H_j has a singular one. This will be made more explicit below.

Next we present the $1D$ Hamiltonians for which anomalous transport has been analyzed rigorously [8, 2]. They are constructed by inverse theory as Jacobi matrices with self-similar fractal spectrum 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 real function such that its restrictions $S|_{I^1_{0,1}} : I^1_{0,1} \to I^0$ are bijective with smooth inverse and such that $S(I^0 \backslash (I_0^1 \cap I_1^1)) \cap I^0 = \emptyset$. The inverse images $S^{-N}(I^0)$ consist of 2^N intervals of generation N. Corresponding to a one-sided code $\sigma = (\sigma_i)_{i\geq 1}$ of 0's and 1's, each of them is denoted by $I_\sigma^N = S_{\sigma_1}^{-1} \circ \ldots \circ S_{\sigma_N}^{-1}(I^0)$. Finally S is supposed to be expansive such that the lengths of the generation intervals I_σ^N decrease exponentially in N uniformly in σ. Now $J = \bigcap_{N\geq 0} S^{-N}(I^0)$ is a fractal and S-invariant set.

A S-invariant ergodic measure μ on J is given by pull-back under the coding map of a shift-invariant ergodic measure on the code space. If μ is moreover a Gibbs measure, then its generalized dimensions are known to exist and to be analytic in q (see [19] and references therein):

$$D_\mu(q) \;=\; \lim_{q\to q'} \frac{1}{q'-1} \lim_{\epsilon\to 0} \frac{\log\left(\int d\mu(E)\, \mu([E-\epsilon, E+\epsilon])^{q'-1}\right)}{\log(\epsilon)}\;, \qquad q \in \mathbf{R}\;. \tag{4}$$

Furthermore, the measure μ is exactly scaling, namely the pointwise dimensions $d_\mu(E) = \lim_{\epsilon\to 0} \log(\mu([E-\epsilon, E+\epsilon]))/\log(\epsilon)$ exist μ-almost surely and are μ-almost surely equal to $\dim_{\rm H}(\mu) = D_\mu(1)$ [19, 8].

Associated to μ is a family $(P_n)_{n\geq 0}$ of orthonormal polynomials satisfying a three-term recurrence relation with real coefficients $(t_n, v_n)_{n\geq 0}$:

$$EP_n(E) \;=\; t_{n+1}P_{n+1}(E) + v_nP_n(E) + t_nP_{n-1}(E)\;, \qquad P_{-1} = 0\;.$$

The coefficients $(t_n, v_n)_{n\geq 0}$ define a three-diagonal symmetric finite-difference Hamiltonian acting on $\ell^2(\mathbf{N})$. It is the Jacobi matrix with self-similar spectral measure μ, its local density of states.

In this work, we shall focus on two examples for both of which μ is constructed with the Bernoulli measure with equal weights on the code space. A uniform Cantor set is obtained using the map $S(E) = |\lambda E| - \lambda + 1$, $\lambda > 2$; the thermodynamics of μ are flat, that is $D_\mu(q) = \log(2)/\log(\lambda)$ for all $q \in \mathbf{R}$. The second family of examples are real Julia sets associated to $S(E) = E^2 - \lambda$, $\lambda > 2$. The thermodynamics of μ is then non-trivial, and the corresponding Jacobi matrix, also called a Julia matrix, now has an exact renormalization property in physical space and its matrix elements t_n are given by a limit-periodic sequence which can be calculated from a simple recurrence relation while the v_n's vanish [4, 3, 5].

The results on quantum transport are the following. For a real Julia matrix H, Mantica has derived and numerically verified [16] that

$$\beta^+_\alpha(H) \;=\; D_\mu(1-\alpha)\;, \qquad \alpha > 0\;. \tag{5}$$

A rigorous proof of $D_\mu(1) \leq \beta^+_\alpha(H) \leq D_\mu(1-\alpha)$ for $\alpha \in (0, \alpha_c(\lambda)]$ with some $\alpha_c(\lambda) > 2$ is given in [8, 2] (more precisely, the upper inequality was shown to hold only for $\beta^+_\alpha(H,\psi)$ where $\psi = |0\rangle$ is the state completely localized at the border of the one-sided lattice; it can, however, be directly verified that $\beta^+_\alpha(H) = \beta^+_\alpha(H,|0\rangle)$). For Julia matrices, transport is hence solely determined by spectral properties. In particular, the intermittency, notably the fact that $\alpha \mapsto \beta^+_\alpha(H)$ is a strictly increasing curve, is due to the non-trivial thermodynamis of the spectral measure.

For uniform Cantor sets, the transport properties can be analyzed numerically [7, 16] and bounds on the dynamics can also be proved [8, 2]. We do not give analytical formulæ here because the theory is not yet satisfactory, nevertheless, the motion is clearly intermittent in the above sense and furthermore $\beta^+_0(H)$ is strictly bigger than $\dim_{\mathrm{H}}(\mu)$. Thermodynamics of the spectrum cannot be at the origin of this, the reason are rather decay properties of the generalized eigenfunctions [16]. It has been suggested [12] that the gap between $\beta^+_0(H)$ and $\dim_{\mathrm{H}}(\mu)$ is in general related to an exponent characterizing the multifractal properties of the generalized eigenfunctions.

Hence we dispose of $1D$ Hamiltonians with intermittent anomalous transport due either to the thermodynamics of the spectral measures or to non-trivial scaling of the generalized eigenfunctions. Using (1) this leads to higher dimensional models with the same transport properties. Our analysis of their spectral properties is based on the following theorem which is a direct corollary of the results in [10].

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

$$\dim_{\mathrm{H}}(\mu_1^{\eta_1} * \ldots * \mu_D^{\eta_D}) \;=\; \min\left\{1\;,\;\sum_{j=1}^{D}\dim_{\mathrm{H}}(\mu_j)\right\}\;, \tag{6}$$

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

Let us give some further explanations of the theorem and sketch its proof. On the right hand side of (6), $\dim_{\rm H}(\mu_j)$ can be replaced by $\dim_{\rm H}(\mu_j^{\eta_j})$ because the mapping $E \mapsto E/\eta_j$ is bi-Lipschitz and therefore does not change the Hausdorff dimensions and pointwise dimensions (that is, $d_{\mu_j^{\eta_j}}(\eta_j E) = d_{\mu_j}(E)$). It is clear that the theorem cannot be true for all $\eta_1, \ldots, \eta_D$ because of resonance phenomena. For example [11], if one considers the convolution of two balanced Bernoulli measures on the same uniform Cantor set, it can be shown that the Fourier transform does not vanish at infinity because of recurrences. Hence the convolution measure cannot be absolutely continuous by the Riemann-Lebesgue lemma even if the Hausdorff dimensions of the two measures sum up to more than 1.

For the proof of the theorem, one notes that $\mu_1^{\eta_1} * \ldots * \mu_D^{\eta_D}$ is the image of the product measure $\mu_1 \otimes \ldots \otimes \mu_D$ under the one-dimensional projection $P_\eta : \mathbf{R}^D \to \mathbf{R}$ given by $P_\eta(E_1, \ldots, E_D) = \sum_{j=1}^D \eta_j E_j$ where $\eta = (\eta_1, \ldots, \eta_D)$. Now it is shown in [10] 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 $\min\{1, \dim_{\rm H}(\nu)\}$ for Lebesgue almost all directions η. Actually [10] 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 [18] generalizing those of [17]. The second statement of the theorem follows similarly from [10].

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

Theorem *Let $\mu_1, \ldots, \mu_D$ be balanced Bernoulli measures on real Julia sets and $H_1, \ldots, H_D$ their Jacobi matrices. Then the Hamiltonian H^η defined in* (1) *as well as its spectral measure μ^η satisfy for Lebesgue almost all $\eta = (\eta_1, \ldots, \eta_D) \in \mathbf{R}_+^D$:*

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

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

(iii) $\beta_\alpha^+(H^\eta) \leq \max_{j=1\ldots D} D_{\mu_j}(1-\alpha)$ *and* $\beta_\alpha^+(H^\eta) \geq \dim_{\rm H}(\mu^\eta)/D$.

Analogous results can be obtained if the μ_j's are Gibbs measures on a Cantor set. However, the upper bounds on the diffusion exponents then contain the more complicated expressions given in [8, 2].

Let us consider the concrete example of a Julia set for which $\dim_{\rm H}(\mu) = D_\mu(1) \approx 1/3$. 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 very slightly bigger than imposed by Guarneri's lower bound $\beta_2(H) \geq 1/D = 1/3$. We further dispose of $3D$ models with absolutely continuous spectrum and a diffusion exponent taking an arbitrary value in the interval $[0.3342, 1]$.

In this example constructed with Julia matrices, the reason for the gap between $\beta_2(H)$

and $\dim_{\rm H}(\mu)/D$ is the intermittency of the transport in the $1D$ model which in turn is due to non-trivial thermodynamics of the spectral measures. Actually an intermittant lower bound $\beta_\alpha^- \geq D_\mu(1/(1+\alpha))/D$ generalizing Guarneri's bound can be obtained in a general framework [9]. For Jacobi matrices associated to measures on Cantor sets and probably also for realistic models for $3D$ quasicrystals, the above gap is certainly also related to decay properties of the generalized eigenfunctions [16, 12].

References

[1] M. Aizenman, S. Molchanov, Commun. Math. Phys. **157**, 245-278 (1993); and M. Aizenman, Rev. Math. Phys. **6**, 1163-1182 (1994).

[2] J.-M. Barbaroux, H. Schulz-Baldes, *Anomalous transport in presence of self-similar spectra*, to appear in Annales Inst. H. Poincaré, Nov. 1999.

[3] M. Barnsley, J. Geronimo, J. Harrington, Commun. Math. Phys. **99**, 303-317 (1985).

[4] J. Bellissard, D. Bessis, P. Moussa, Phys. Rev. Lett. **49**, 701-704 (1982).

[5] J. Bellissard, *Stability and Instability in Quantum Mechanics* in *Trends and developments in the Eighties*, S. Albeverio & Ph. Blanchard Eds, (World Scientific Pub. Co., Singapore, 1985),

[6] I. Guarneri, Europhys. Lett. **10**, 95-100 (1989); Europhys. Lett. **21**, 729-733 (1993).

[7] I. Guarneri, G. Mantica, Phys. Rev. Letters **73**, 3379-3383 (1994).

[8] I. Guarneri, H. Schulz-Baldes, *Upper bounds for quantum dynamics governed by Jacobi matrices with self-similar spectra*, to appear in Rev. Math. Phys., Nov 1999.

[9] I. Guarneri, H. Schulz-Baldes, *Intermittant lower bound on quantum diffusion*, preprint 1999.

[10] X. Hu, S. J. Taylor, Math. Proc. Camb. Phil. Soc. **115**, 527-544 (1994).

[11] J. P. Kahane, R. Salem, *Ensembles Parfaits et Séries Trigonometriques*, (Hermann, Paris, 1963).

[12] R. Ketzmerick, K. Kruse, S. Kraut, T. Geisel, Phys. Rev. Lett. **79**, 1959-1962 (1997).

[13] Y. Last, private communication.

[14] P. A. Lee, T. V. Ramakrishnan, Rev. Mod. Phys. **57**, 287-337 (1985).

[15] D. Mayou, in *Lectures on quasicrystals*, edited by F. Hippert, D. Gratias (Les Editions de Physique, Les Ulis, 1994).

[16] G. Mantica, Physica **D 103**, 576-589, (1997); Physica **D 109**, 113-127 (1997).

[17] J. M. Marstrand, Proc. London Math. Soc. **4**, 257-302 (1954).

[18] P. Mattila, Ann. Acad. Sci. Fenn. Ser. A I Math. **1**, 227-244 (1975).

[19] Y. Pesin, *Dimension Theory in Dynamical Systems*, (The University of Chicago Press, 1997).

[20] F. Piéchon, Phys. Rev. Letters **76**, 4372-4375 (1996).

[21] S. Roche, T. Fujiwara, Phys. Rev. **B 58**, 11338-11344 (1998).

[22] H. Schulz-Baldes, J. Bellissard, Rev. Math. Phys. **10**, 1-46 (1998); J. Stat. Phys. **91**, 991-1027 (1998).

[23] B. Simon, Commun. Math. Phys. **176**, 713-722 (1996).

[24] C. Sire, Europhys. Lett. **10**, 483-488 (1989).

[25] C. Sire and D. Gratias, in NATO ASI Series B: Physics Vol. 319, edited by P. Turchi and A. Gonis, 127-154, (Plenum Press, New York and London, 1994).

[26] J. Vidal, R. Mosseri, J. Bellissard, J. Phys. **A 32**, 2361-2367 (1999).