Intermittent lower bound on quantum diffusion

Italo Guarneri[1], Hermann Schulz-Baldes[2]

[1] Universita di Como, 7 via Lucini, 22100 Como, Italy

[2] TU Berlin, FB Mathematik, Straße des 17. Juni 136, 10623 Berlin, Germany

Abstract

An intermittent lower bound on quantum diffusion is proven in presence of a multifractal spectral measure.

1 Introduction

Lower bounds on quantum diffusion by fractal properties of the spectral measures were first proven by the first named author [4]. Considerable refinements are due to Combes [2], Last [12], Kiselev and Last [11] and ourselves [7]. These results state that the algebraic growth exponents in time of positive moments of the position operator are bounded below by dimensional properties of the LDOS (local density of states), possibly improved by taking into account the asymptotic behavior of the generalized eigenfunctions.

Numerical calculations and theoretical investigations have shown that one-dimensional quantum dynamics may exhibit non-trivial growth exponents for moments of the position operator, and that such exponents, scaled to the moment order, are typically different for moments of different order [5, 14, 13]. This *multi-scaling* phenomenon was termed *quantum intermittency* in [5]. Moreover, intermittency has been related to the multifractal properties of the LDOS [13]. Evidence supporting a similar link between averaged wave packet propagation and multifractal properties of the density of states has been given for the Fibonacci and the Harper Hamiltonians [14]. A first mathematical analysis of this phenomenon was given in [1], where intermittent upper bounds on certain toy models were proven. Using similar large deviation techniques, we prove in this work a completely general intermittent lower bound in terms of the generalized dimensions of the LDOS, which is valid under the only assumption that the latter dimensions exist. Although we formulate it within a one-dimensional framework, it can be directly transposed as in [12, 15, 7] to the higher dimensional case.

We acknowledge financial support of the SFB 288.

2 Statement of the result

We consider a self-adjoint, bounded Hamiltonian H acting on the Hilbert space $\ell^2(\mathbf{N})$. The canonical base is denoted by $(|n\rangle)_{n\in\mathbf{N}}$. The unbounded position operator on $\ell^2(\mathbf{N})$ is defined by $X|n\rangle = n|n\rangle$. We are interested in studying the spreading of a wave packet initially localized at $|0\rangle$ under the quantum dynamics generated by H, and we analyse it with help of the moments of the time-averaged probability distribution on $\mathbf{N}$, notably the time-averaged expectation values of powers of X. Our aim is to characterize the spreading by properties of the spectral measure μ of H with respect to $|0\rangle$.

We recall the definition of the generalized (or multifractal) dimensions of the spectral measure μ by (for $q \neq 0$)

$$D_\mu(q) \;=\; \frac{\tau_\mu(q)}{q-1} \;=\; \frac{1}{q-1} \lim_{T\to\infty} \frac{\log(\int d\mu(E)\, \mu(B_{1/T}(E))^{q-1})}{\log(1/T)} \;, \tag{1}$$

and $B_{1/T}(E)$ is the ball of size $1/T$ around $E \in \mathbf{R}$ and the latter limit is supposed to exist.

The diffusion exponents $\beta_q^\pm$, $q \neq 0$, are defined as the growth exponents

$$\beta_q^- \;=\; \liminf_{T\to\infty} \frac{\log(M_q(T))}{\log(T^q)} \;, \qquad \beta_q^+ \;=\; \limsup_{T\to\infty} \frac{\log(M_q(T))}{\log(T^q)} \;, \tag{2}$$

of the time-averaged moments of the position operator:

$$M_q(T) \;=\; \sum_{n\geq 0} n^q \int_0^T \frac{dt}{T}\, |\langle n|e^{-\imath tH}|0\rangle|^2 \;. \tag{3}$$

We recall that all diffusion exponents lie in the interval $[0,1]$ if the off-diagonal elements of the Hamiltonian H fall off sufficiently rapidly. Finally, the diffusion exponents are non-decreasing, continuous functions of q, except possibly at $q = 0$.

Theorem *Suppose that the generalized dimensions exist for all $q \in \mathbf{R}$ and are finite for some $q < 1$. The following inequality then holds for all $q > 0$:*

$$\beta_q^- \;\geq\; D_\mu\left(\frac{1}{1+q}\right) \;.$$

Remark 1: The generalized dimensions exist for all the Gibbs measures of hyperbolic dynamical systems, hence in particular for the IFS measures considered in [6, 1].

Remark 2: It is possible to improve our lower bound in the spirit of [10, 11] whenever further information about the generalized eigenfunctions is given. More precisely, let the generalized eigenfunctions P_n be defined via functional calculus by

$$\langle n|f(H)|0\rangle \;=\; \int d\mu(E)\, P_n(E)\, f(E) \;, \qquad f \in C_0(\mathbf{R}) \;,$$

and suppose that there exists a $\gamma \in \mathbf{R}$ such that for all E in the spectrum of H the bound

$$\sum_{n\leq N} P_n(E)^2 \;\leq\; c\, N^\gamma \;, \qquad c \in \mathbf{R} \;, \tag{4}$$

holds for all $N \in \mathbf{N}$. Then an improvement of the proof below shows that $\beta_q^- \geq D_\mu(1-q/\gamma)/\gamma$. If now γ is small and the thermodynamics of μ is important so that $D_\mu(q)$ increases considerably for negative q, this bound can be better than the above. Actually such a γ exists and can be calculated for $1D$ quasicrystals [8]. However, it turns out to be rather large. This results from the hypothesis that (4) holds uniformly in energy. More detailed analysis of the link between a local exponent $\gamma(E)$ and the spectral properties near E was made by Jitormiskaya and Last [9].

3 Proof of the result

First we remark that algebraic growth exponents of time averages are equal to growth exponents of gaussian averages:

Lemma *Let f be a non-negative measurable function satisfying $f(t) \leq Ct^n$ for some $C > 0$ and $n \geq 0$. Then*

$$\liminf_{T\to\infty} \frac{\log\left(\int_0^T dt\, f(t)\right)}{\log(T)} \;=\; \liminf_{T\to\infty} \frac{\log\left(\int_0^\infty dt\, e^{-t^2/4T^2} f(t)\right)}{\log(T)} \;.$$

Similar equalities hold for $\limsup$ *and other growth exponents.*

Proof: Let α and β denote the exponents on the left and right hand side respectively. The inequality

$$\int_0^T dt\, f(t) \;\leq\; e^4 \int_0^\infty dt\, e^{-t^2/4T^2} f(t)$$

implies that $\alpha \leq \beta$. On the other hand, we have

$$\begin{aligned}\int_0^\infty dt\, e^{-t^2/4T^2} f(t) \;&\leq\; \int_0^{T^{1+\epsilon}} dt f(t) \;+\; C\int_{T^{1+\epsilon}}^\infty dt\, e^{-t^2/4T^2} t^n \\ &\leq\; \int_0^{T^{1+\epsilon}} dt f(t) \;+\; C' e^{-T^\epsilon/4} T^n \;.\end{aligned}$$

This implies that $\beta \leq (1+\epsilon)\alpha$ for any $\epsilon > 0$. □

Hence we shall prove a lower bound on the gaussian mean. Moreover we note that $t \mapsto \langle n|e^{-\imath tH}|0\rangle$ is a symmetric function, so that we can symmetrize time and gaussian means. Then we translate the problem of proving a lower bound to that of proving an upper bounds on presence probability, notably, for any $N(T) \geq 0$, we have:

$$\begin{aligned}&\sum_{n\geq 0} n^q \,\frac{1}{2T\sqrt{\pi}} \int_{-\infty}^\infty dt\; e^{-t^2/4T^2}\, |\langle n|e^{-\imath tH}|0\rangle|^2 \\ &\geq\; N(T)^q \sum_{n>N(T)} \frac{1}{2T\sqrt{\pi}} \int_{-\infty}^\infty dt\; e^{-t^2/4T^2}\, |\langle n|e^{-\imath tH}|0\rangle|^2 \\ &=\; N(T)^q \left(1 - \sum_{n\leq N(T)} \frac{1}{2T\sqrt{\pi}} \int_{-\infty}^\infty dt\; e^{-t^2/4T^2}\, |\langle n|e^{-\imath tH}|0\rangle|^2\right) \;.\end{aligned}$$

In order to prove an upper bound on the second expression in the parenthesis, we split the wave packet as in [12] in a small, fast diffusing part, and in a rest, but we make this splitting time dependent as in [7]. For a given real Borel set I, let χ_I denote its indicator function and set $|\psi_I\rangle = \chi_I(H)|0\rangle$. We choose, for a given $\alpha \in \mathbf{R}$,

$$I(T) \;=\; \left\{ E \in \mathbf{R} \;\middle|\; \int d\mu(E')\, e^{-(E-E')^2 T^2} < T^{-\alpha} \right\} \;,$$

so that the large deviation bound (11) gives $\|\psi_{I(T)}\|^2 = \mu(I(T)) \approx T^{f_\mu(\alpha)-\alpha}$. Using the decomposition $|0\rangle = |\psi_{I(T)}\rangle + |\psi_{I(T)^c}\rangle$, we then obtain:

$$\frac{1}{2T\sqrt{\pi}} \sum_{n \le N(T)} \int_{-\infty}^{\infty} dt\; e^{-t^2/4T^2} |\langle n|e^{-\imath tH}|0\rangle|^2 \;\le\; 1 - \|\psi_{I(T)}\|^2 + A(T) + B(T) \;,$$

where

$$A(T) \;=\; \frac{1}{2T\sqrt{\pi}} \sum_{n \le N(T)} \int_{-\infty}^{\infty} dt\; e^{-t^2/4T^2} |\langle n|e^{-\imath tH}|\psi_{I(T)}\rangle|^2 \;,$$

and

$$B(T) \;=\; \frac{1}{T\sqrt{\pi}} \Re e \sum_{n \le N(T)} \int_{-\infty}^{\infty} dt\; e^{-t^2/4T^2} \langle n|e^{-\imath tH}|\psi_{I(T)}\rangle\; \langle \psi_{I(T)^c}|e^{\imath tH}|n\rangle \;.$$

Let us now first calculate and bound $A(T)$:

$$\begin{aligned} A(T) \;&=\; \sum_{n \le N(T)} \int_{I(T)} d\mu(E) \int_{I(T)} d\mu(E')\; P_n(E) P_n(E')\, e^{-(E-E')^2 T^2} \\ &\le\; \sum_{n \le N(T)} \int_{I(T)} d\mu(E)\, |P_n(E)|^2 \int_{I(T)} d\mu(E')\; e^{-(E-E')^2 T^2} \\ &\le\; T^{-\alpha} \sum_{n \le N(T)} \int_{I(T)} d\mu(E)\, |P_n(E)|^2 \;. \end{aligned} \tag{5}$$

Using the inequality $2P_n(E)P_n(E') \le P_n(E)^2 + P_n(E')^2$, we obtain similarly a bound $B(T) \le B_1(T) + B_2(T)$ where

$$\begin{aligned} B_1(T) \;&=\; \sum_{n \le N(T)} \int_{I(T)} d\mu(E) \int_{I(T)^c} d\mu(E')\; |P_n(E)|^2\, e^{-(E-E')^2 T^2} \\ &\le\; T^{-\alpha} \sum_{n \le N(T)} \int_{I(T)} d\mu(E)\, |P_n(E)|^2 \;. \end{aligned} \tag{6}$$

and

$$B_2(T) \;=\; \sum_{n \le N(T)} \int_{I(T)} d\mu(E) \int_{I(T)^c} d\mu(E')\; |P_n(E')|^2\, e^{-(E-E')^2 T^2} \;. \tag{7}$$

In order to bound $\int_{I(T)} d\mu(E)\, e^{-(E-E')^2 T^2}$ for $E' \in I(T)^c$, we introduce

$$E_l \;=\; \sup\{E \in I(T)\,|\, E < E'\} \;, \qquad E_r \;=\; \inf\{E \in I(T)\,|\, E > E'\} \;.$$

Then $\int_{I(T)} d\mu(E)\, e^{-(E-E')^2T^2}$ is bounded above by

$$\int_{I(T)\cap(-\infty,E_l]} d\mu(E)\, e^{-(E-E_l)^2T^2} + \int_{I(T)\cap[E_r,\infty)} d\mu(E)\, e^{-(E-E_r)^2T^2} \;\leq\; 2T^\alpha \;.$$

Now we can accomplish the proof of the theorem. For that purpose, we bound $A(T)$, $B_1(T)$ and $B_2(T)$ by replacing the domains of intergration $I(T)$, $I(T)$ and $I(T)^c$ in (5), (6) and (7) respectively by $\mathbf{R}$. As the generalized eigenfunctions are normalized, one thus obtains

$$A(T) + B_1(T) + B_2(T) \;\leq\; c\,T^{-\alpha}\,N(T) \;.$$

Thus we get:

$$\sum_{n\geq 0} n^q\, \frac{1}{2T\sqrt{\pi}} \int_{-\infty}^{\infty} dt\; e^{-t^2/4T^2}\, |\langle n|e^{-\imath tH}|0\rangle|^2 \;\geq\; N(T)^q(\mu(I(T)) - c\,T^{-\alpha}\,N(T)) \;.$$

Now the large deviation bound (11) implies that for any $\delta > 0$ there exists a positive constant $C(\delta) < \infty$ such that $\mu(I(T)) \geq C(\delta)T^{f_\mu(\alpha)-\alpha-\delta}$. Finally we choose $N(T) = T^{f_\mu(\alpha)-\delta}C(\delta)/2c$. This choice assures the positivity of the right hand side in the latter equation. Thus we obtain:

$$\sum_{n\geq 0} n^q\, \frac{1}{2T\sqrt{\pi}} \int_{-\infty}^{\infty} dt\; e^{-t^2/4T^2}\, |\langle n|e^{-\imath tH}|0\rangle|^2 \;\geq\; \frac{C(\delta)}{2}\, T^{(q+1)f_\mu(\alpha)-\alpha-(q+1)\delta} \;.$$

Up to now $\alpha \in \mathbf{R}$ was arbitrary. Maximising the right hand side over $\alpha \in \mathbf{R}$ and taking the limit $\delta \to 0$, one gets the theorem.

Appendix: Large deviation theory for singular measures

Here present the form of multifractal analysis used in the above proof. It is directly based on the Gärtner-Ellis large deviation theorem [3] which we reproduce for the convenience of the reader. Recall that by definition a point $x \in \mathbf{R}$ is an exposed point of a real function Λ^* if there exists a $\lambda \in \mathbf{R}$, called the exposing hyperplane of x, such that

$$\lambda y - \Lambda^*(y) \;>\; \lambda x - \Lambda^*(x) \;, \qquad \forall\;\; y \neq x \;.$$

Theorem [3] *Let $(A_t)_{t\in\mathbf{R}_+}$ be a family of real random variables on a probability space $(\Omega, \mathbf{P})$. Their characteristic functions are defined as*

$$\Lambda_t(\lambda) \;=\; \log\left(\int d\mathbf{P}(\omega)\, e^{\lambda A_t(\omega)}\right) \;, \qquad \lambda \in \mathbf{R} \;.$$

We suppose that for all $\lambda \in \mathbf{R}$ the following limit exists:

$$\Lambda(\lambda) \;=\; \lim_{t\to\infty} \frac{1}{t}\Lambda_t(t\lambda) \;, \tag{8}$$

and further that Λ is finite in a neighborhood of 0. *Then Λ is a convex function and so is its Legendre transform Λ^*.*

(i) For any closed set $F \subset \mathbf{R}$, one has

$$\limsup_{t\to\infty} \frac{1}{t} \log(\mathbf{P}(\{A_t \in F\})) \;\leq\; -\inf_{x\in F} \Lambda^*(x) \;. \tag{9}$$

(ii) For any open set $G \subset \mathbf{R}$, we have

$$\liminf_{t\to\infty} \frac{1}{t} \log(\mathbf{P}(\{A_t \in G\})) \;\geq\; -\inf_{x\in G\cap\mathcal{F}} \Lambda^*(x) \;, \tag{10}$$

where $\mathcal{F}$ is the set of exposed points of Λ^* having an exposing hyperplane in the interior of the set $\{\lambda \in \mathbf{R} \,|\, \Lambda(\lambda) < \infty\}$.

We want to analyse the fractal properties of probability measure μ on $\mathbf{R}$ with the large deviation theory in $(\mathbf{R}, \mu)$. Herefore we study the random variables

$$A_t(E) \;=\; \frac{\log(\int d\mu(E')\, e^{-(E-E')^2 e^{-2t}})}{t} \;.$$

Under the hypothesis that the appearing limits exist, the associated rate function is the Legendre transform of

$$\begin{aligned}
\Lambda(\lambda) \;&=\; \lim_{t\to\infty} \frac{1}{t} \log\left(\int d\mu(E)\, \left(\int d\mu(E')\, e^{-(E-E')^2 e^{-2t}}\right)^{-\lambda}\right) \\
&=\; \lim_{T\to\infty} \frac{\log\left(\int d\mu(E)\, \left(\int d\mu(E')\, e^{-(E-E')^2 T^2}\right)^{-\lambda}\right)}{\log(T)} \;.
\end{aligned}$$

Actually the function Λ is linked to $\tau_\mu(q)$ and $D_\mu(q)$ as defined in (1) by:

$$\Lambda(\lambda) \;=\; \lambda D_\mu(1-\lambda) \;=\; -\tau_\mu(1-\lambda) \;, \qquad \Lambda^*(x) \;=\; x - f_\mu(x) \;,$$

where f_μ is the scaling function of the measure μ defined to be the Legendre transform of τ_μ. To see this, let us show $\tau_\mu(q) = -\Lambda(1-q)$ for all $q \in \mathbf{R}\backslash\{0\}$. As the characteristic function on a ball of size $1/T$ used in the definition (1) is less or equal to the function $ee^{-(E-E')^2T^2}$, the inequalities $\tau_\mu(q) \leq -\Lambda(1-q)$ for $q < 1$ and $\tau_\mu(q) \geq -\Lambda(1-q)$ for $q > 1$ follow immediately. For the converse, we note that any $\epsilon > 0$:

$$\int d\mu(E')\, e^{-(E-E')^2T^2} \;\leq\; \int d\mu(E')\, \chi(|E-E'| \leq T^{-1+\epsilon}) + 2e^{-T^\epsilon} \;.$$

This implies that $(1-\epsilon)\tau_\mu(q) \geq -\Lambda(1-q)$ for $q < 1$ and $(1-\epsilon)\tau_\mu(q) \leq -\Lambda(1-q)$ for $q > 1$.

Under the hypothesis that $D_\mu(q) < \infty$ for some $q < 0$, we can now dispose of the above large deviation bounds. In particular, for the sets $\{A_t > \alpha\}$, $\alpha \geq f_\mu(\alpha)$, the lower bound implies that:

$$\liminf_{T\to\infty} \frac{\log\left(\mu\left(\left\{E \in \mathbf{R} \,\middle|\, \int d\mu(E') e^{-(E-E')^2T^2} < T^{-\alpha}\right\}\right)\right)}{\log(T)} \;\geq\; f_\mu(\alpha) - \alpha \;. \tag{11}$$

References

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

[2] J.-M. Combes, *Connection between quantum dynamics and spectral properties of time evolution operators*, in *Differential Equations with Applications to Mathematical Physics*, Ames W.F., Harell E.M., Herod J.V. Eds, Academic Press, Boston (1993).

[3] A. Dembo, O. Zeitouni, *Large Deviation Techniques and Applications*, (Jones and Barlett, Boston, London, 1993).

[4] I. Guarneri, *Spectral properties of quantum diffusion on discrete lattices*, Europhys. Lett., **10**, 95-100, (1989); *On an estimate concerning quantum diffusion in the presence of a fractal spectrum*, Europhys. Lett., **21**, 729-733, (1993).

[5] I. Guarneri, G. Mantica, *Multifractal Energy Spectra and Their Dynamical Implications*, Phys. Rev. Lett. **73**, 3379-3383 (1994).

[6] 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.

[7] I. Guarneri, H. Schulz-Baldes, *Lower bounds on wave packet propagation by packing dimensions of spectral measures*, Elect. J. Math. Phys. **5**, (1999).

[8] B. Iochum, L. Raymond, D. Testard, *Resistance of one-dimensional quasicrystals*, Physica **A 187**, 353-368 (1992).

[9] S. Jitorminskaya, Y. Last, *Dimensional Hausdorff properties of singular continuous spectra*, Phys. Rev. Lett. **76**, 1765-1769 (1996).

[10] R. Ketzmerick, K. Kruse, S. Kraut, T. Geisel, *What Determines the Spreading of a Wave Packet?*, Phys. Rev. Lett. **79**, 1959-1962 (1997).

[11] A. Kiselev, Y. Last, *Solutions, spectrum, and dynamics for Schrödinger operators on infinite domains*, preprint, mp-arc 99-206.

[12] Y. Last, *Quantum dynamics and decomposition of singular continuous spectra*, J. Funct. Anal. **142**, 402-445 (1996).

[13] G. Mantica, *Quantum intermittency in almost periodic systems derived from their spectral properties*, Physica **D 103**, 576-589, (1997); *Wave Propagation in Almost-Periodic Structures*, Physica **D 109**, 113-127 (1997).

[14] F. Piéchon, *Anomalous Diffusion Properties of Wave Packets on Quasiperiodic Chains*, Phys. Rev. Lett. **76**, 4372-4375 (1996).

[15] H. Schulz-Baldes, J. Bellissard, *Anomalous transport: a mathematical framework*, Rev. Math. Phys. **10**, 1-46 (1998).