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On an Estimate Concerning Quantum Diffusion in the Presence of a Fractal Spectrum.

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Abstract. – An inequality is proven, relating the rate of spreading of wave packets to the information dimension of the spectrum. This result makes use of a new and general definition of the growth exponent based on discrete Mellin transforms, and corrects an erroneous statement in a previous proof of a similar estimate.

Studies on quantum transport in crystals and quasi-crystals at low temperature have brought into light a connection between singular continuous energy spectra and quantum diffusion. Multifractal energy spectra have been identified in various models for the motion of quantum particles over one-dimensional discrete lattices [1-3] and the corresponding long-time behaviour of wave packets has been found to be diffusive, with the mean-square displacement of the particle increasing asymptotically as some power of time more or less close to one. Some quite general results about this connection between spectral properties and asymptotic dynamical properties can be derived within the mathematical framework of spectral theory. In ref. [4] it was pointed out that a singular spectrum is actually a *necessary* condition in order that the «growth exponent» may be less than 2 in the 1-dimensional case. How the precise value of this exponent is related to the fractal structure of the spectrum is still an open question, though some heuristic arguments indicate that it should be equal to twice the fractal (Hausdorff) dimension [2,4] as indeed it was found (within numerical accuracy) in the hitherto investigated cases. Although for a different asymptotic parameter a precise relation to generalized dimension has been found [5], to the best of the author's knowledge the only exact result about the growth exponent is still the lower bound established in ref. [4], according to which this exponent cannot be less than twice the information dimension of the spectral measure of the diffusing state; this type of bound is also discussed and generalized in ref. [6].

The first problem in the way of a rigorous analysis of the growth exponent is that of giving a clean definition of the exponent itself. In this paper such a definition is given, using analytical tools which have been extensively used for other purposes in the study of singular measures [7]. This new definition allows for a more precise formulation of the lower bound of ref. [4], which is here proven afresh to hold for any initial state as soon as the corresponding spectral measure satisfies a certain assumption. The new proof substantially improves the

previous one, which implicitly assumed a special choice of the state but was erroneously claimed to have a more general validity in ref. [4].

Let \mathcal{H} be a separable Hilbert space, $B = \{e_n\}_{n \in \mathbf{N}}$ a complete orthonormal set of vectors of \mathcal{H} , and U a unitary operator in \mathcal{H} with a purely continuous spectrum. For $\psi \in \mathcal{H}$ and integer t let

$$\psi_n(t) = \langle e_n | U^t \psi \rangle.$$

Then it is known that

$$\lim_{t \rightarrow \infty} \overline{|\psi_n|^2}_t \equiv \lim_{t \rightarrow \infty} t^{-1} \sum_{s=1}^t |\psi_n(s)|^2 = 0.$$

Therefore in some sense the distribution $p_n(t) = \overline{|\psi_n|^2}_t$ spreads over the base B , and its 2nd moment, *i.e.* the quantity

$$\mathcal{G}_B(t) = \sum_1^\infty n^2 p_n(t)$$

diverges to $+\infty$ in the limit $t \rightarrow \infty$. Let

$$\mathcal{D}_B = \left\{ \psi \in \mathcal{H}, \sum_1^\infty n^2 |\langle e_n | \psi \rangle|^2 < +\infty \right\}$$

and assume that

$$\mathcal{A}_B = \bigcap_{t=-\infty}^{+\infty} U^t(\mathcal{D}_B) \neq \{0\}.$$

If $\psi \in \mathcal{A}_B$ the 2nd moment is finite for all t (in the following the suffix B will be dropped whenever not strictly necessary). A very convenient means for investigating the long-time behaviour of the 2nd moment (and of other quantities to be defined below) is provided by a discretized version of the Mellin transform [7], which is formally defined for complex β as follows:

$$Z(\beta, \psi) = \sum_{t=1}^\infty t^{-\beta-1} \mathcal{G}(\psi, t). \quad (1)$$

If the series in eq. (1) converges for $\beta = \beta_0$, then it converges $\forall \beta$ such that $\text{Re}(\beta) > \text{Re}(\beta_0)$; if it diverges for $\beta = \beta_0$, then it diverges $\forall \beta$, so that $\text{Re}(\beta) < \text{Re}(\beta_0)$. A growth exponent $\bar{\beta}_2(\psi)$ for the 2nd moment can then be defined as the infimum of the real β 's such that the series converges. Likewise, $\forall \alpha > 0$ one can define a growth exponent $\bar{\beta}_\alpha$ for the α -th moment. The basic tool of this paper is still another growth exponent $\bar{\beta}_0$, which is defined for *any* state ψ as follows. For $\varepsilon \in (0, 1)$ let

$$\bar{n}(\varepsilon, \psi, t) = \min \left\{ n: \sum_{k \geq n} p_k(t) < \varepsilon \|\psi\|^2 \right\}.$$

This function has the following properties: 1) \bar{n} is non-decreasing for $\varepsilon \rightarrow 0$; 2) $\bar{n} \rightarrow \infty$ for $t \rightarrow \infty$, because all the $p_n(t)$ tend to 0 in that limit due to the continuity of the spectrum; 3) the Chebyshev inequality, which holds if $\psi \in \mathcal{A}_B$:

$$\bar{n}(\varepsilon, \psi, t) \leq \varepsilon^{-1/2} \mathcal{G}^{1/2}(\psi, t) \|\psi\|^{-1}. \quad (2)$$

A Mellin transform can be defined for \bar{n} , too:

$$W(\beta, \varepsilon, \psi) = \sum_{t=1}^{\infty} t^{-\beta-1} \bar{n}^2(\varepsilon, \psi, t).$$

The transform W has properties similar to those of $Z(\beta, \psi)$. In particular, a convergence abscissa $\bar{\beta}(\varepsilon, \psi)$ can be defined. Since \bar{n} is non-decreasing as $\varepsilon \rightarrow \infty$, it follows that $\bar{\beta}(\varepsilon, \psi)$ is itself non-decreasing; then let

$$\bar{\beta}_0(\psi) = \lim_{\varepsilon \rightarrow 0} \bar{\beta}(\varepsilon, \psi) = \sup_{0 < \varepsilon < 1} \bar{\beta}(\varepsilon, \psi).$$

For $\psi \in \mathcal{A}_B$ the Chebyshev inequality (2) yields $\bar{\beta}_0(\psi) \leq \bar{\beta}_2(\psi)$.

In order to estimate $\bar{\beta}_0(\psi)$ one has to estimate the decay of the distribution $p_n(t)$. To this end the following result will be used:

Lemma 1. – Let $\psi \in \mathcal{H}$ and let $\theta(\delta)$ be a real function tending to 0 in the limit $\delta \rightarrow 0^+$, such that $\forall t \in \mathbf{N}$, $\mu(I) < \theta(\delta_t)$ for any interval I of length less than δ_t , where μ is the spectral measure of ψ and $\delta_t = 2\pi t^{-1}$. Then $\forall t$, $n \in \mathbf{N}$

$$p_n(t) \leq c\theta(2\pi t^{-1}) \ln t,$$

with c a constant independent of ψ .

This result was proven in ref. [4] (eq. (5)). \diamond

In order to obtain an explicit form for the function θ , one has to investigate the scaling properties of the spectral measure μ . Let us assume that the local scaling index

$$\gamma(x) = \lim_{\delta \rightarrow 0} \frac{\log(\mu(I_{\delta, x}))}{\log \delta} \tag{3}$$

exists for μ -almost all points x in the support of the spectral measure, $I_{\delta, x}$ being an interval of width δ centred at x ; moreover, let us assume that

$$\gamma(x) = \bar{\gamma} = \text{const } \mu\text{-a.e.} \tag{4}$$

Under assumption (4) $\bar{\gamma}$ can be identified with the *information dimension* of the spectrum. Although assumption (4) guarantees that the measure of «most» small spectral intervals scales as $\delta^{\bar{\gamma}}$, it still does not ensure that the function $\theta(\delta) = \delta^{\bar{\gamma}}$ will satisfy the hypothesis of lemma 1, because the limit (3) may not be uniform over the whole spectrum. Nevertheless, an «approximately uniform» scaling is enforced by the following:

Lemma 2. – Under assumption (4), $\forall \eta \in (0, 1)$ and $\forall \gamma \in (0, \bar{\gamma})$, a subset $J_{\eta, \gamma}$ of $[0, 2\pi]$ and a positive constant $C_{\eta, \gamma}$ can be found, such that

- i) $\mu(J_{\eta, \gamma}) > 1 - \eta$,
- ii) $\forall t \in \mathbf{N}$ and $\forall x \in J_{\eta, \gamma}$, $\mu(I_t(x)) < C_{\eta, \gamma} \delta_t^{\bar{\gamma}}$, where $I_t(x)$ is an interval of width $\delta_t = 2\pi/t$ centred at x .

The proof is obtained by taking the limit (3) over the sequence δ_t and by applying Egorov's theorem [8]. \diamond

The announced estimate on the growth exponents can now be obtained by applying lemma 1 to the spectral component ψ_{η} of the wave packet ψ which belongs in the «large»

subset J_γ ; indeed, the following result shows that for small enough γ the whole wave packet has to spread at least as fast as that component.

Theorem. – Let the spectral measure of a vector $\psi \in \mathcal{H} \setminus \{0\}$ satisfy assumption (4). Then $\bar{\beta}_0(\psi) \geq 2\bar{\gamma}$, and if moreover $\psi \in \mathcal{A}_B \setminus \{0\}$, then also $\beta_2(\psi) \geq 2\bar{\gamma}$.

Proof. – Given $\gamma \in (0, \bar{\gamma})$, $\eta > 0$ and ψ , with $\|\psi\| = 1$, define ψ_γ as the spectral projection of ψ over the set J_γ defined in lemma 2 (the suffix γ is not essential here); then $\phi_\gamma = \psi - \psi_\gamma$ is orthogonal to ψ_γ , and

$$\|\psi_\gamma\|^2 + \|\phi_\gamma\|^2 = 1.$$

For any integer n_0 ,

$$\sum_{n > n_0} \overline{|\psi_n|^2} = \sum_{n > n_0} \overline{|\psi_{\gamma, n}|^2} + \sum_{n > n_0} \overline{|\phi_{\gamma, n}|^2} + 2 \operatorname{Re} \sum_{n > n_0} \overline{(\psi_{\gamma, n}^* \phi_{\gamma, n})} t.$$

The last term is easily seen to be $\leq 2\|\psi_\gamma\|\|\phi_\gamma\|$, so that

$$\sum_{n > n_0} \overline{|\psi_n|^2} \geq \sum_{n > n_0} \overline{|\psi_{\gamma, n}|^2} - 2\|\psi_\gamma\|\|\phi_\gamma\|. \quad (5)$$

Now $\|\psi_\gamma\|$ can be made arbitrarily close to 1 by choosing a small enough γ . In particular, given ε , one can choose γ so small that

$$\varepsilon \|\psi_\gamma\|^2 - 2\|\psi_\gamma\| \sqrt{1 - \|\psi_\gamma\|^2} > \frac{\varepsilon}{2}.$$

With γ chosen in this way, the last inequality together with (5) and with the definition of $\bar{n}(\psi_\gamma, \varepsilon, t)$ entails that if $n_0 < \bar{n}(\psi_\gamma, \varepsilon, t)$, then

$$\sum_{n > n_0} \overline{|\psi_n|^2} > \frac{\varepsilon}{2}, \quad (6)$$

i.e. that $\bar{n}(\varepsilon/2, \psi, t) > n_0$ if $n_0 < \bar{n}(\varepsilon, \psi_\gamma, t)$. Thus $\bar{\beta}(\varepsilon/2, \psi) \geq \bar{\beta}(\varepsilon, \psi_\gamma)$, whence $\bar{\beta}_0(\psi) \geq \bar{\beta}(\varepsilon, \psi_\gamma)$. In order to estimate $\bar{\beta}(\varepsilon, \psi_\gamma)$ notice that for the vector ψ_γ the function θ of Lemma 1 is provided by Lemma 2 in the form

$$\theta(\delta) = C_{\gamma, \gamma} \delta^\gamma,$$

so that for any integer n_0

$$\sum_{n=1}^{n_0} \overline{|\psi_{\gamma, n}|^2} \leq c(2\pi)^\gamma C_{\gamma, \gamma} n_0 t^{-\gamma} \log t,$$

which implies that

$$\bar{n}(\psi_\gamma, \varepsilon, t) \geq c' t^\gamma (\log t)^{-1}$$

with c' a constant depending on ε . Therefore, $\bar{\beta}(\varepsilon, \psi_\gamma) \geq 2\gamma$. Since $\bar{\beta}_0(\psi)$ has been proved above to be $\geq \bar{\beta}(\varepsilon, \psi_\gamma)$, it must satisfy the same inequality; moreover, since the latter holds $\forall \gamma < \bar{\gamma}$ it must also hold for $\gamma = \bar{\gamma}$. The last statement in the thesis is an immediate consequence of the Chebyshev inequality. \diamond

Remarks. – 1) Under such general assumptions the possibility cannot be excluded that the various growth exponents be infinite. Further assumptions concerning the operator U and the base B are needed in order to obtain upper estimates for these exponents [9].

2) The above result holds not only for strictly (multi)fractal measures but even for classical ones. In particular, with absolutely continuous spectra one has $\bar{\beta}_0 \geq 2$.

3) According to available numerical studies, the actual growth exponent can be significantly larger than the above lower bound [9].

4) Mellin transforms may prove much more effective than shown here. For example, the actual growth of the 2nd moment as a function of time sometimes displays an oscillatory behaviour superimposed on the average power law behaviour [9], and the period of such oscillations increases exponentially in time. An analysis of the *complex* singularities Z may account for this behaviour, as in previous applications of the Mellin transform [7].

* * *

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