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## Spectral Properties of Quantum Diffusion on Discrete Lattices (\*).

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**Abstract.** – The possibility of quantum diffusion over discrete lattices is discussed on the ground of general spectral theory, in connection with the problem of quantal suppression of classical chaos. Given the Hausdorff dimension of the spectrum, an asymptotic lower bound for the spreading of wave packet can be established. This bound shows that diffusive spread over one- and quasi one-dimensional lattices can take place only if the spectrum is singular continuous.

Many problems in quantum physics lead quite naturally to investigate the asymptotic properties in time of the propagation of wave packets on discrete lattices. Examples of specific interest to the present paper are the tight-binding models (with random potentials) of solid-state physics and the kicked-rotator (KR) model, which has attracted much attention in connection with studies on quantum chaos [1, 2]. While the lattice in tight-binding models is directly related to a periodic structure in physical space, in the KR model lattice sites correspond to the angular-momentum eigenstates of a rotator, and hopping between them is induced by  $\delta$ -like «kicks» occurring periodically in time. In both cases, classical analogy would suggest that under certain conditions the quantum motion is diffusive, in the sense that the average distance travelled by the «particle» on the lattice is asymptotically proportional to the square root of time. The existence of quantum diffusion is a physically important question, because in tight-binding models diffusion is closely related to conductivity [3] and in the KR model to the role of classical chaos in quantum mechanics.

In spite of classically grounded expectations, diffusion turns out to be absent in both models, at least in the case of one-dimensional lattices. Far from being accidental, this analogy between so different models could be traced back to a nontrivial similarity of their

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mathematical formalism [4, 5], and the quantum effect which is responsible for the absence of diffusion is now called localization in both cases (Anderson localization in the former, «dynamical» localization in the latter).

Whereas Anderson localization could be rigorously proved, this is not yet the case for dynamical localization, which was nevertheless demonstrated by a huge amount of numerical results and by the above hinted formal analogy with the Anderson model. Anyway, as soon as it became clear that the quantum KR would never reproduce the classical unbounded diffusion, Chirikov, Izrailev and Shepelyansky put forward a heuristic argument (henceforth referred to as the Siberian argument) which yielded a remarkable estimate of the localization length in the KR [6], very well confirmed by numerical experiments [7, 8].

Even though this estimate is now generally accepted, it is not so commonly realized that the argument behind it has actually a wider scope. As a matter of fact, it is a spectral argument for the absence of diffusion in dynamical models, and actually a very general one. The present paper is aimed at mathematically substantiating this point by means of a simple result of spectral analysis.

It is well known that wave packets have no chance to diffuse in the absence of a continuous spectrum, and that, conversely, a continuous spectral component enforces unbounded propagation [9]. In the one-dimensional case, the asymptotic nature of the propagation will range between two extreme cases, according to the nature of the spectrum. The first is just localization, and corresponds to a pure-point spectrum. The second is «ballistic» motion, with the distance growing proportional to time, and corresponds to an absolutely continuous spectrum (in the KR model this is known as quantum resonance).

The point of the present paper is that intermediate asymptotic regimes, in which the wave packet spreads more slowly, are connected with spectra of a peculiar nature. It will be shown, first heuristically in the spirit of the Siberian argument, and then rigorously, that quantum diffusion on a one-dimensional lattice is possible only if the spectrum has a singular component, *i.e.*, one of zero (Lebesgue) measure.

Were «singular» the same as «pure point», one would be forced to conclude that diffusion is utterly impossible. Therefore the Siberian argument falls short of providing a complete, though heuristic, proof of the absence of diffusion on one-dimensional lattices only because it cannot exclude the occurrence of a singular *continuous* spectrum<sup>(1)</sup>. This kind of a spectrum has become of interest in solid-state physics in connection with investigations on incommensurate structures [11]. Though its mathematical aspects have been analyzed in detail [12], its physical relevance is not yet completely clear. Singular continuous spectra are a quite common occurrence for Hamiltonians on quasi-periodic lattices (see ref. [13-15] for recent results in this vein); on the other hand, it has been argued that singular continuous spectra may be scarcely relevant to the problem of localization in tight-binding models of the Anderson type, on account of their unstable nature [10]. The possibility of using the results of the present paper as an argument for the absence of diffusion in dynamical models depends on whether a likewise negative attitude is taken towards singular continuous spectra in the context of dynamical localization. Anyway, it must be emphasized that these results are of a very general nature and can be applied to any problem in which the propagation of wave packets on a lattice can be described by a unitary group in discrete time (*e.g.*, tight-binding models and systems subjected to external perturbations periodic in time). Moreover, they have a straightforward generalization to quasi-one-dimensional

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<sup>(1)</sup> As discussed in ref. [10], a similar shortcoming occurred with a well-known and far-reaching approach to one-dimensional Anderson localization.

lattices, *i.e.* to lattices that can be obtained by associating a fixed number of sites to each place in a one-dimensional array.

Let the evolution of a quantum system with states in some separable Hilbert space  $\mathcal{H}$  be defined by a discrete unitary group  $\{\hat{S}^t\}$  where  $t$  is an integer-valued time variable and the unitary operator  $\hat{S}$  describes the evolution over a fixed interval of real time (*e.g.*, a period of some time-periodic external perturbation). Let a complete orthonormal basis  $\{e_n\} (-\infty < n < +\infty)$  be given in  $\mathcal{H}$ . Then the evolution of any state vector  $\psi \in \mathcal{H}$  can be identified with the propagation of a wave packet on the integer lattice by putting  $\psi_n(t) = \langle e_n | \hat{S}^t \psi \rangle$ . It will be assumed that, if

$$d^2(t) = \sum_{n=-\infty}^{+\infty} n^2 |\psi_n(t)|^2 < +\infty$$

at some time  $t$ , then  $d^2(t) < +\infty$  at any other time  $t$ .

The heuristic part of the argument runs as follows. Let the wave packet at  $t=0$  be concentrated at the site 0, *i.e.*  $\psi = e_0$ , and suppose that it will asymptotically diffuse, *i.e.* that  $d^2(t) \sim \text{const} \cdot t$  for  $t \rightarrow \infty$ . Since the spectral measure of  $\psi$  is the Fourier transform of the correlation function  $R(t) = \langle \hat{S}^t \psi | \psi \rangle$ , by performing a finite Fourier transform of  $R(t)$  ( $0 \leq t \leq T$ ), one will be able to resolve the spectrum of  $\hat{S}$  down to a scale  $\sim T^{-1}$ . The number of points thus determined in the spectrum will have the meaning of an effective number of frequencies appearing in the motion up to time  $T$ , and can be identified, in order of magnitude at least, with  $d(T)$ , which measures the spread of the wave packet at the same time  $T$ . Therefore, asymptotically as  $T \rightarrow \infty$  the spectrum is resolved, on a scale  $T^{-1}$ , by a number of points  $\sim \text{const} \cdot T^{1/2}$ , which implies that the measure of the spectrum is zero and that its fractal dimension is 1/2.

A similar conclusion can be obtained rigorously as follows. Consider an observable of the form

$$\hat{O} = \sum_{n=-\infty}^{+\infty} \phi(|n|) |e_n\rangle \langle e_n|, \quad (1)$$

where  $\phi(n)$  is a positive nondecreasing function, and suppose that the domain of  $\hat{O}$  is invariant under the action of  $\hat{S}$ . For  $x \geq 0$  denote by  $\nu(x)$  the number of sites  $n$  such that  $\phi(|n|) \leq x$ . Finally, let the spectral projections of  $\hat{S}$  be  $\hat{E}_\lambda$  ( $0 \leq \lambda \leq 2\pi$ ), so that the spectral measure of  $\psi$  is  $d\mu(\lambda) = d\|\hat{E}_\lambda \psi\|^2$ . It will be assumed that  $\mu$  is a continuous measure, because the point of interest here is unbounded propagation, in which a point spectrum cannot contribute. A result on the asymptotics for large  $T$  of

$$\langle\langle \hat{O} \rangle\rangle_T = T^{-1} \sum_{t=0}^T \langle \hat{S}^t \psi | \hat{O} | \hat{S}^t \psi \rangle$$

will now be proved:

**PROPOSITION.** – Let  $\eta(\delta)$  be a continuous nondecreasing function in  $[0, \delta_0]$ , with  $0 < \delta_0 \leq 2\pi$  and  $\eta(0) = 0$  such that  $\mu(\Delta) \leq \eta(\delta)$  for all intervals  $\Delta \subset [0, 2\pi]$  of length  $\delta < \delta_0$ . Then, for sufficiently large  $T$  and  $\forall x > 0$ ,

$$\langle\langle \hat{O} \rangle\rangle_T \geq x[1 - c_1 \nu(x) \eta(2\pi T^{-1}) \ln T] \quad (2)$$

with  $c_1$  a suitable constant.

The proof consists in estimating the decay of time averages of the coefficients  $\psi_n(t)$ . Let  $\mathcal{H}_0$  be the closed subspace of  $\mathcal{H}$  spanned by  $\hat{S}^t \psi$ ,  $-\infty < t < +\infty$  and  $\hat{P}$  the associated projector. Let  $\psi_0$  be a generating vector for  $\hat{S}$  in  $\mathcal{H}_0$  ( $\psi$  itself is one such vector, but later we shall need some freedom in the choice of  $\psi_0$ ). Then,  $\forall k$  one has [16]

$$\hat{P}e_k = \int_0^{2\pi} f_k(\lambda) d\hat{E}_\lambda \psi_0$$

with  $f_k(\lambda)$  such that

$$\int_0^{2\pi} |f_k(\lambda)|^2 d\mu(\lambda) = \|\hat{P}e_k\|^2 \leq 1. \quad (3)$$

Then

$$\psi_k(t) = \int_0^{2\pi} \tilde{f}_k(\lambda) \exp[i\lambda t] d\mu(\lambda)$$

and, denoting time averages up to time  $T$  by  $\langle \cdot \rangle_T$ ,

$$\begin{aligned} \langle |\psi_k^2| \rangle_T &= \int_0^{2\pi} d\mu(\lambda) \int_0^{2\pi} d\mu(\lambda') \frac{1 - \exp[i(\lambda - \lambda')(T+1)]}{T(1 - \exp[i(\lambda - \lambda')])} \tilde{f}_k(\lambda) f_k(\lambda') \leq \\ &\leq \int_0^{2\pi} d\mu(\lambda) |f_k(\lambda)|^2 \int_0^{2\pi} d\mu(\lambda') \frac{|\sin[((\lambda - \lambda')(T+1))/2]|}{T|\sin[(\lambda - \lambda')/2]|}. \end{aligned} \quad (4)$$

Let  $I_\lambda$  be the inner integral in (4). In order to estimate it, we introduce a variable  $x = \lambda' - \lambda$  ( $-\pi \leq x \leq \pi$ ) and use  $|\sin(x/2)| \geq |x| \pi^{-1}$  for the denominator in the integrand. There are  $2\nu_T + 1 \leq 2 + T$  zeros of  $\sin(x(T+1)/2)$  in  $[-\pi, +\pi]$  and these zeros define a partition of  $[-\pi, +\pi]$  in subintervals of length  $< 2\pi T^{-1}$ . If  $T$  is large enough, the measure  $\mu$  of any such interval will be  $\leq \gamma(2\pi T^{-1})$ . Upon writing  $I_\lambda$  as a sum of integrals over all such intervals one gets the following straightforward estimate:

$$I_\lambda \leq 2\pi(1 + T^{-1}) \gamma(2\pi T^{-1}) \left[ 1 + \sum_{k=1}^{\nu_T} \frac{1}{2k\pi} \right] \leq c_1 \gamma(2\pi T^{-1}) \ln T$$

with a suitable constant  $c_1$ . Substituting this into (4) one gets

$$\langle |\psi_k^2| \rangle_T \leq c_1 \gamma(2\pi T^{-1}) \ln T. \quad (5)$$

From (1) and the last estimate it follows that,  $\forall x > 0$

$$\langle\langle \hat{O} \rangle\rangle_T \geq x \sum_{(n)} \langle |\psi_n^2| \rangle_T$$

the sum being understood over all  $n$ 's such that  $\phi(|n|) \geq x$ . Therefore, recalling (5) and the definition of  $\nu(x)$ , one gets the announced estimate.

The above proposition can be used to get an asymptotic lower bound for the time average of the expectation of the square  $d^2$  of the distance travelled by a «particle» on a lattice of given dimension. For that, one must first reorder the lattice sites in a one-dimensional array

according to nondecreasing values of their distance from the starting site. One can then define  $\phi(n)$  as the squared distance of the  $n$ -th site from the starting point (in the original lattice). All relevant information about the geometry of the original lattice will then be embodied in the function  $\nu(x)$ ; for example,

$$\nu(x) \sim \alpha_1 x^{1/2}$$

for a one- (or quasi-one-) dimensional lattice, and

$$\nu(x) \sim \alpha_2 x$$

for a two-dimensional lattice. In order to obtain an explicit form for the function  $\gamma(\delta)$ , let us suppose that the spectrum has Hausdorff dimension  $\alpha \leq 1$  in the following precise sense: the measure  $\mu$  is supported by a set  $\Omega \subset [0, 2\pi]$  of Hausdorff dimension  $\alpha$ , and  $\mu(A) = 0$  for any subset  $A$  of  $\Omega$  of dimension  $< \alpha$ . Then  $\mu$  will be absolutely continuous with respect to the Hausdorff measure  $h_\alpha$  on  $\Omega$  of dimension  $\alpha$ , and one can take

$$\gamma(\delta) = \text{const } \delta^\alpha$$

as soon as the density  $w$  of  $\mu$  relative to  $h_\alpha$  is (essentially) bounded. On the other hand, the latter condition can always be satisfied by a suitable choice of the generating vector (g.v.)  $\psi_0$ . Indeed, if  $w$  is unbounded, one can define a new bounded density by  $w' = cw$  for  $w \leq 1$  and  $w' = c$  for  $w > 1$ , with  $c$  a normalizing factor. The measures  $\mu, \mu'$  with densities  $w, w'$  are mutually absolutely continuous; therefore, a g.v. can be found [16], whose spectral measure is  $\mu'$ .

After fulfilling such preliminary constructions (2), yields for the one- or quasi-one-dimensional case:

$$\langle d^2 \rangle_T \geq x(1 - c_2 x^{1/2} T^{-\alpha} \ln T)$$

for  $\forall x > 0$ ; hence,

$$\langle d^2 \rangle_T \geq c_3 \frac{T^{2\alpha}}{\ln^2 T}$$

(with  $c_2, c_3$  appropriate constants). It is then seen that diffusion is possible only if  $\alpha \leq 1/2$ , for otherwise the packet would spread too fast. In particular, in the case of an absolutely continuous spectrum ( $\alpha = 1$ ) the last estimate says that  $\langle d^2 \rangle_T$  will grow faster than  $T^{2-\varepsilon}$  for any  $\varepsilon$ , and this is consistent with known results for the «resonant» KR [17].

The natural question, whether the necessary condition  $\alpha \leq 1/2$  just established can be turned into a sufficient one, will not be entered here. I just wish to mention that useful hints in this connection are provided by some classical results in Fourier analysis, because the coefficients  $\psi_k(t)$ , whose decay in time determines the asymptotic nature of the motion, are the Fourier-Stieltjes coefficients of the measure  $\int f_k(\lambda) d\mu(\lambda)$ . It is a known result [18] that it is always possible to find a measure supported by a Cantor set of dimension  $\alpha < 1$  such that its Fourier-Stieltjes coefficients are of order  $t^{-(\alpha/2-\varepsilon)}$  for any  $\varepsilon > 0$ ; this yields an indication that  $\alpha = 1/2$  may also be a sufficient condition for diffusion.

In the case of a 2-dimensional lattice, by inserting in (2) the appropriate  $\nu(x)$  one gets

$$\langle d^2 \rangle_T \geq c_4 \frac{T^\alpha}{\ln T}$$

which does not any more exclude asymptotic diffusion in the presence of an absolutely continuous spectrum. It appears therefore that the simple spectral argument discussed above does not give so effective indications in the higher-dimensional case, as it did in the one-dimensional one.

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