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LETTER TO THE EDITOR

Quantum diffusion and lack of universal one-parameter scaling in one-dimensional disordered lattices with long-range coupling

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Abstract. It is generally believed that all eigenstates in one-dimensional disordered lattices are localized provided disorder is uncorrelated. We show that this statement fails for a one-dimensional Anderson model with a special type of long-range inter-site interaction, resulting in a specific, non-parabolic quasi-particle energy dispersion. Remarkably, the states appearing to be delocalized belong to the tail of the band.

In their pioneering work, Mott and Twose raised the statement that in one dimension (1D) all the states of random systems become exponentially localized upon introducing any amount of disorder [1]. Later on, Abrahams *et al* [2] confirmed this belief by introducing the one-parameter scaling theory of localization, extending the Mott–Twose conclusion to two-dimensional (2D) systems as well (see [3, 4] for a comprehensive review). This viewpoint was dominant in the physics community by the end of the 1980s and the beginning of the 1990s, until it was found that extended states may appear in 1D random systems upon introducing either short-range [5–10] or long-range [11, 12] correlations in the disorder. Suppression of localization by correlations was further used for the explanation of the high conductivity of doped polyaniline [8] as well as the transport properties of random semiconductor superlattices [13].

In this letter we demonstrate that extended states may appear in *one dimension* even for moderately large *uncorrelated* diagonal disorder and, moreover, in the band *tails*, despite the usual belief that states deep in the band tails are localized [3]. The crucial peculiarity responsible for such unusual behaviour is the long-range inter-site interaction, resulting in a specific eigenenergy dispersion law. In short, it appears that the level spacing decreases on increasing the system size in the same manner (or even slower) than the degree of disorder reduced by the quasi-particle motion (see equation (4) below). Therefore, if the disorder is of a *perturbative* magnitude for a given lattice size, it will remain *perturbative* on increasing the size, consequently excluding quasi-particle localization.

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We consider a tight-binding model Hamiltonian on a regular lattice of length N with diagonal disorder:

$$\mathcal{H} = \sum_n \epsilon_n |n\rangle\langle n| + \sum_{mn} J_{nm} |n\rangle\langle m| \tag{1}$$

where $|n\rangle$ is the ket vector of a state with energy ϵ_n, with n being integers in the interval $-N/2 \leqslant n \leqslant N/2$, with N even. The hopping integrals J_{mn} are chosen to be of the form $J_{nm} = J/|n-m|^\alpha$ ($J_{nn} \equiv 0$), where J is the coupling between nearest-neighbour (NN) sites in the lattice and $\alpha > 0$. Note that for $\alpha = 3$, the Hamiltonian (1) describes 1D Frenkel excitons [14]. In what follows, we will restrict ourselves to the range $1 < \alpha \leqslant \frac{3}{2}$, adopting this limitation only in order to demonstrate numerically our theoretical reasoning. In the conclusion we will discuss qualitatively some realistic models in two and three dimensions where it is not necessary to assume such a restriction.

In the model we will be dealing with, the source of disorder is the stochastic fluctuations of the energies ϵ_n from site to site. Their distribution is chosen to be uniform within an interval of size Δ: $P(\epsilon_n) = 1/\Delta$ for $|\epsilon_n| \leqslant \Delta/2$ and $P(\epsilon_n) = 0$ otherwise, thus having the variance $\langle\epsilon_n^2\rangle = \Delta^2/12$. The quantity Δ will be referred to as the degree of disorder. We do not assume any correlation in the energy fluctuation of different sites, so the joint distribution function of a realization of disorder is $\prod_n P(\epsilon_n)$.

In order to substantiate our reasoning, we assume periodic boundary conditions and rewrite (1) in the Bloch-waves representation, which are the eigenstates of the off-diagonal part of $\mathcal{H}$:

$$\mathcal{H} = \sum_K E_K |K\rangle\langle K| + \sum_{KK'} (\delta\mathcal{H})_{KK'} |K\rangle\langle K'| \tag{2a}$$

where $K \equiv 2\pi k/N$ runs over the first Brillouin zone, with k being integers in the interval $-N/2 \leqslant k < N/2$. Here E_K is the unperturbed eigenenergy

$$E_K = J \sum_{n\neq 0} \frac{1}{|n|^\alpha} \mathrm{e}^{\mathrm{i}Kn} = 2J \sum_{n=1}^{\infty} \frac{1}{n^\alpha} \cos Kn \tag{2b}$$

and $(\delta\mathcal{H})_{KK'}$ is the inter-mode coupling matrix

$$(\delta\mathcal{H})_{KK'} = \frac{1}{N} \sum_n \epsilon_n \mathrm{e}^{\mathrm{i}(K-K')n}. \tag{2c}$$

As has been shown in [15, 16], coupling to far neighbours yields non-perturbative effects on the quasi-particle eigenenergies close to the edges of the band even for $\alpha = 3$. It is reasonable to expect larger effects when $\alpha < 3$. Therefore, we keep the long-range terms in (2b) due to their important role in what we will be dealing with. It is a matter of simple analysis to show that in close proximity to the centre of the band $K = 0$, the energy spectrum takes the form

$$E_K \simeq 2J\zeta(\alpha) - JA|K|^{\alpha-1} \qquad |K| \ll 1 \tag{3}$$

where $\zeta(\alpha) = \sum_{n=1}^{\infty} n^{-\alpha}$ is the Riemann ζ-function and we have defined the constant $A \equiv 2\Gamma(2-\alpha)\cos[\pi(\alpha-1)/2]/(\alpha-1)$.

Depending on the degree of disorder and the lattice size, the operator $\delta\mathcal{H}$ may couple the extended states $|K\rangle$ to each other, thus resulting in their localization. Our task now is to calculate the typical fluctuation of this matrix in order to gain insight into the magnitude of the state mixing. The corresponding magnitude of interest is $\sigma_{KK'}^2 = \left\langle |(\delta\mathcal{H})_{KK'}|^2 \right\rangle$, where the angular brackets indicate the average over the distribution $\prod_n P(\epsilon_n)$. After performing the average in $(2c)$ one finds

$$\sigma_{KK'} \equiv \sigma = \frac{\Delta}{\sqrt{12N}} \tag{4}$$

for any value of N and K, K'. Here σ is referred to as the *effective* degree of disorder. As we can see, the typical magnitude of the state mixing scales as $N^{-1/2}$, manifesting the well known exchange narrowing effect [17]: the effective degree of disorder for an extended state is reduced by a factor $\sqrt{N}$ relative to the seeding value Δ. The scaling found should be compared with that of the eigenenergy spacing deduced from equation (3). Let us now suppose that $\alpha \leqslant \frac{3}{2}$. Then, the eigenenergy separation close to the band centre δE scales as $N^{1-\alpha}$, with $1-\alpha \geqslant -\frac{1}{2}$, meaning that the effective degree of disorder σ goes down upon increasing the system length N in the same manner as or faster than the energy separation δE. This finding has a dramatic effect on the localization properties of the states with small K. Indeed, even if one starts with a *non-perturbative* magnitude of Δ in the sense that $\sigma \gg \delta E$ (at a fixed lattice size), so that the states are mixed by the disorder and thus are localized, they become not mixed (delocalized) for larger system lengths because of the faster dropping of the effective degree of disorder σ compared to the energy spacing δE.

The results of numerical diagonalization of the Hamiltonian (1) for bounded chains of different lengths are summarized in figures 1–3. They unambiguously confirm our qualitative arguments. To examine the character of the eigenfunctions (localized or extended) we have calculated their inverse participation ratio (IPR), according to the standard definition (see, e.g., [16])

$$I_\nu = \sum_n |\Psi_{\nu n}|^4 \tag{5}$$

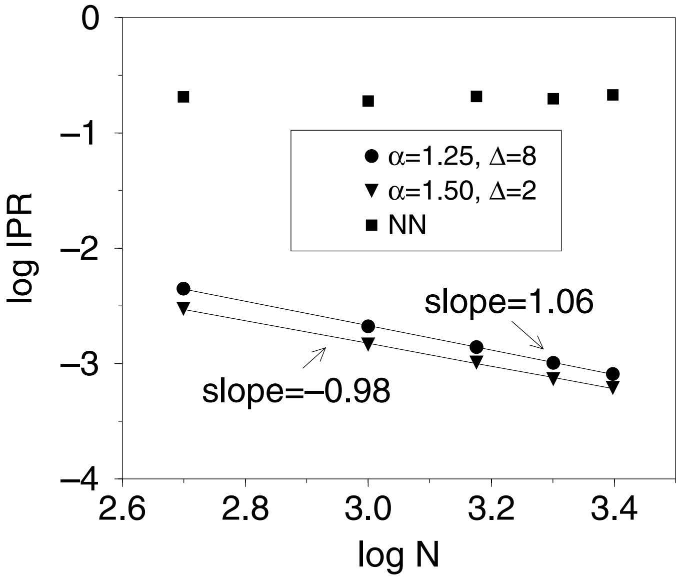

Figure 1. IPR scaling of the uppermost eigenfunction obtained by diagonalization of the Hamiltonian (1) and averaging over 20 realizations of the disorder. Results corresponding to random systems with long-range interaction for $\alpha = \frac{5}{4}$ and $\Delta = 8$ (circles) and $\alpha = \frac{3}{2}$ and $\Delta = 2$ (triangles) are compared with those obtained within the NN approximation for $\Delta = 2$ (squares).

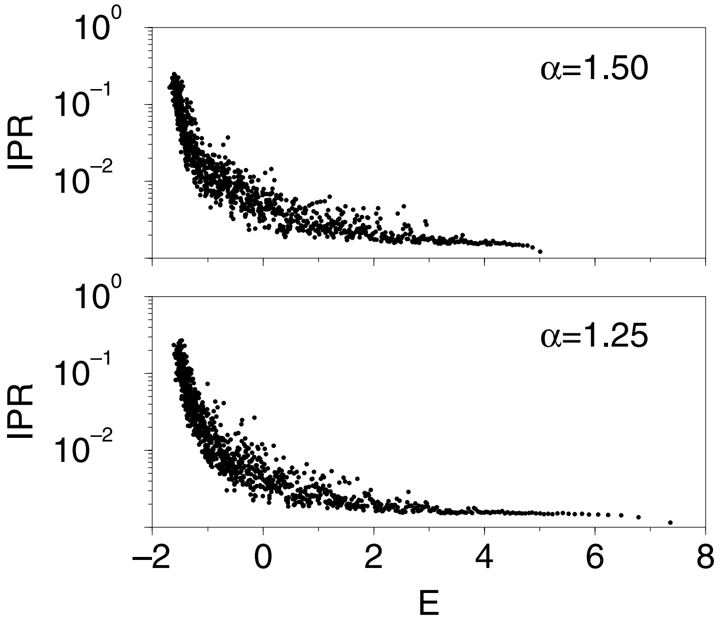

Figure 2. Plot of the IPR as a function of energy for two values of α with $N = 1000$ and $\Delta = 0.5$. It can be seen that there is a mobility edge at roughly $E \approx -0.5$, separating extended and localized states.

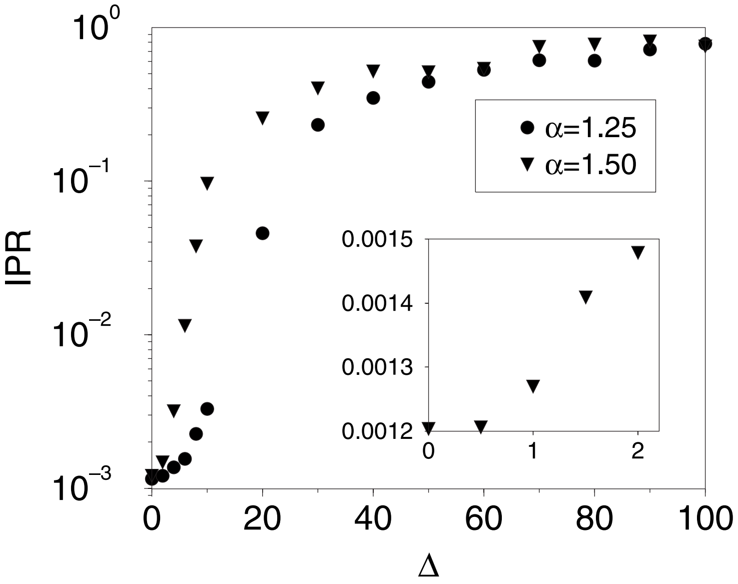

Figure 3. IPR of the uppermost eigenfunction as a function of the degree of disorder Δ for a chain of length $N = 1000$. Circles and triangles represent the results for $\alpha = \frac{5}{4}$ and $\frac{3}{2}$, respectively, obtained by averaging over 20 realizations of disorder. The inset shows an enlarged view of the IPR at a small degree of disorder for $\alpha = \frac{3}{2}$. The occurrence of a continuous Anderson transition is clearly seen.

where the sum runs over lattice sites and it is assumed that the eigenfunction $\Psi_{\nu n}$ of the νth eigenstate is normalized to unity. On increasing the length N, the IPR scales as N^{-1} for delocalized states, which are spread uniformly over the system. In contrast, localized states exhibit much higher values: the higher the value, the smaller the localization length, with it finally being unity for the extreme case of localization at a single site. In fact, the participation ratio I_ν^{-1} is of the order of the number of sites over which an eigenfunction is spread. The IPR of the uppermost eigenstate is shown in figure 1 as a function of the chain length N, when the interaction between all sites is taken into account for $\alpha = \frac{3}{2}$ and $\frac{5}{4}$ as well as within the NN approximation. In what follows we will scale the energy in units of J by taking $J = 1$. The plots comprise the result of 20 averages over disorder realizations. The fact that the slopes of the straight lines in a log–log plot are almost equal to -1 (the theoretical value for an extended state) undoubtedly confirms the extended nature of the uppermost state. Note that the IPR becomes independent of the system size within the NN approximation, in perfect agreement with the statement that those states are localized [1, 2].

Figure 2 displays the IPR for a typical realization of a random chain of length $N = 1000$ for $\alpha = \frac{3}{2}$ and $\frac{5}{4}$. It can clearly be seen that the top states are delocalized for the selected parameters since their IPR are close to the theoretical value of N^{-1}. Far from the top of the band, one observes a steep change of the IPR at about $E \approx -0.5$, where it starts to increase towards the bottom of the band. Note that this change indicates the presence of a mobility edge (only one in the case at hand).

Figure 3 shows that the uppermost state undergoes a continuous Anderson transition as the degree of disorder increases: the IPR calculated as a function of the degree of disorder for a fixed system size ($N = 1000$) goes up upon raising the degree of disorder Δ, clearly indicating the occurrence of the delocalization–localization transition. The states at the top of the band are delocalized for a moderate degree of disorder Δ and become localized at higher values of Δ.

We stress that our findings contradict the one-parameter scaling theory of localization [2] stating that all the states in 1D are localized provided any amount of uncorrelated disorder is introduced in the system. This theory assumes that the dimensionless conductance is the only relevant parameter determining the N-scaling of the energy levels and the subsequent localization properties of the states. From our study, it follows unambiguously that the N-scaling of the disorder may play a dominant role, violating the one-parameter scaling theory and leading to the impossibility of matching our results with this theory.

In summary, we have shown that the statement about weak localization in 1D random systems, i.e. that any amount of disorder results in localization of all eigenstates [1, 2], fails in the range of the quasi-particle spectrum where it scales as a power law in $|K|$ with an exponent smaller than $\frac{1}{2}$. The states lying in such an energy range are delocalized at moderate disorder strength and undergo a continuous Anderson transition as the degree of disorder increases.

To conclude, let us discuss the relevance of our reasoning for more realistic models as compared to that considered in this letter, namely, long-range inter-site coupling in the form $|n - m|^{-\alpha}$ with $1 < \alpha \leqslant \frac{3}{2}$. Let us further stress that it is most important to compare the N-scaling of two basic quantities: the effective degree of disorder, σ, and the energy level spacing, δE. The former always behaves proportionally to $\mathcal{N}^{-1/2} \sim N^{-D/2}$, where $\mathcal{N}$ and N are the D-dimensional volume and lateral sizes of the system, respectively, and D is the dimensionality. The N-scaling of the energy spacing depends on the dimensionality and the inter-site coupling as well as on the spectrum range. Turning to two dimensions ($D = 2$), we will find $\sigma \sim N^{-1}$. Thus, our reasoning relative to the unusual delocalization properties of the eigenstates is applicable to those models in which the energy spectrum scales linearly or sub-linearly in $|\boldsymbol{K}|$. Some planar dipolar systems such as Frenkel excitons [18] and spins in antiferromagnets [19], provide just such a possibility: the energy spectrum in those systems behaves linearly in $|\boldsymbol{K}|$ at small $|\boldsymbol{K}|$. We also might expect the same peculiarity for mid-band states of NN tight-binding models (both 2D and 3D), where the energy always scales linearly with the wavenumber. At least, earlier [20, 21] and recent [22, 23] numerical simulations performed for the mid-band states always showed a clear tendency for the corresponding eigenfunctions to delocalization at moderate disorder. Finally, it is worth mentioning that the electron energy spectrum of 2D electrons in Si-MOSFET structures has a linear term [24], which may be expected to be of importance as the temperature decreases. Then, our findings provide a possible explanation for the metal–insulator transition observed in these structures [25].

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