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Critical Hamiltonians on one-dimensional disordered lattices

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We focus on tight-binding Hamiltonians on a regular one-dimensional lattice with *non-random* long-range inter-site coupling $J_{mn} = J/|m-n|^{\mu}$ and random uncorrelated site energies. Within the model the localization-delocalization transition occurs at one of the energy band edges provided $1 < \mu < 3/2$. Using the model we demonstrate that the ratio of the first two momenta of the participation number distribution for the critical states is a size invariant parameter at some value of the disorder magnitude Δ_c. We claim that the invariance manifests the transition. We find that $\Delta_c \neq 0$ at $1 < \mu < 3/2$, suggesting that the system undergoes the localization-delocalization transition with respect to disorder magnitude. At $\mu \geq 3/2$, all states are localized.

1 Introduction

Since the seminal paper by Anderson forty six years ago [1], the localization-delocalization transition (LDT) of non-interacting quasiparticles in random media has been a topic of extensive studies. For many years the single-parameter scaling theory of localization (STL) was retaining the general belief that all single-particle eigenstates were exponentially localized in one (1D) and two (2D) dimensions [2], and the LDT could occur only in three-dimensional (3D) geometry. Despite the STL does not assume any restriction on the character of disorder, it works well in application to a variety of materials.

Because of recent advances in nanotechnology, researchers have renewed their interest in the LDT in low-dimensional systems, where the interplay between quantum interference and disorder results in peculiarities of the Anderson localization that are not observed in 3D systems. Unexpectedly, at the end of the eighties and beginning of the nineties, several theoretical works [3–6] raised doubts about the generality of the STL conclusions. These works provided clear evidence that short-range correlations in diagonal disorder could cause delocalization of quasiparticles states even in 1D geometry. This fact was put forward to explain the high conductivity of doped polyaniline [5] as well as the transport properties of random semiconductor superlattices [7]. However, it was realized that extended states formed a set of zero measure in the thermodynamic limit, and no signatures of the LDT were found.

Further, it was demonstrated that long-range correlations in diagonal disorder could also act towards delocalization of 1D quasiparticle states [8]. Thus, the spectrum of the 1D Hamiltonians with long-

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range correlated disorder revealed two mobility edges separating extended and localized states [8, 9]. Remarkably, quasiparticles undergo Bloch-like oscillations between these two mobility edges after applying a uniform electric field [10].

Recently, it was argued, both numerically [11] and by making use of the supersymmetric method for disorder averaging combined with the renormalization group approach [12], that a LDT could occur within 1D and 2D models with *uncorrelated* diagonal disorder and *non-random* inter-site coupling which falls according to a power law (see also Ref. [13]). Apart from the importance of this finding from a general point of view, the model is relevant for several physical systems. As an example, let us mention dipolar Frenkel excitons on 2D regular lattices where molecules are subjected to randomness due to a disordered environment [14–16]. Some biological light-harvesting antenna systems can be described by the model [17, 18]. Magnons in 2D disordered spin systems provide one more example of interest [19].

In this paper, we present further progress in the characterization of the LDT in 1D systems subjected to diagonal disorder and *non-random long-range* inter-site interaction. The outline of the paper is as follows. In Sec. 2 we present the model and discuss magnitudes relevant to monitor the LDT. These are the two first momenta of the participation number distribution: the mean and the standard deviation. The results of numerical analysis of size and disorder scaling of these two magnitudes are presented in Sec. 3. The numerical study demonstrates that the ratio of the two momenta is invariant at the transition. We conclude with a brief discussion of the relevance of the results in Sec. 4.

2 Model Hamiltonian

We consider the Anderson Hamiltonian on a 1D regular lattice with N sites

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

The coupling between lattice sites m and n is set in the form $J_{mn} = J/|m-n|^{\mu}$, where $J > 0$ without loss of generality, $J_{nn} \equiv 0$, and the lattice constant is set to unity. We stress that the hopping integrals do not fluctuate, while the on-site energies $\{\varepsilon_n\}_{n=1}^{N}$ are random variables. They are assumed to be uncorrelated for different sites and distributed symmetrically around zero, thus having zero mean, $\langle \varepsilon_n \rangle = 0$. Here $\langle \ldots \rangle$ indicates average over disorder realizations. For performing numerical simulations, we use a box distribution for ε_n with a width Δ and standard deviation $\sigma \equiv \langle \varepsilon_n^2 \rangle^{1/2} = \Delta/\sqrt{12}$. Within this class of Hamiltonians, the LDT (with respect to the disorder magnitude Δ) occurs at the upper energy band edge provided $1 < \mu < 3/2$ [11, 12].

Often the participation number (PN) or its inverse, known as the inverse participation ratio (IPR), is considered to examine the character of eigenfunctions (localized or extended). The PN is defined as follows

$$P_\nu = \left[\sum_{n=1}^{N} |\psi_{\nu n}|^4 \right]^{-1} , \tag{2}$$

where $\psi_{\nu n}$ denotes the nth component of the ν-th normalized eigenstate of the Hamiltonian (1), $|\Psi_\nu\rangle = \sum_{n=1}^{N} \psi_{\nu n} |n\rangle$, with $\nu = 1, \ldots, N$. For a localized state, the PN depends on the localization length and does not depend on the system size, provided the latter is large compared to the localization length. For an extended state, the PN shows scaling with the system size, which is usually put forward as a signature of delocalization. It should be noticed, however, that the statement that a particular eigenstate is indeed delocalized, is physically meaningful only in the thermodynamic limit ($N \to \infty$). Otherwise, one cannot distinguish a truly extended eigenstate from the one with a localization length larger than the system size. In other words, a simple inspection of an eigenstate does not suffice to uncover its nature. Consequently, a study of the size scaling of relevant physical quantities is required.

One of such quantities is the PN (or IPR) distribution function (see, for instance, Refs. [20, 21]). We show numerically in Sec. 3 that at some value of disorder Δ_c, the ratio of the standard deviation of the PN (SDPN) to the mean PN (MPN) is size invariant; the family of SDPN/MPN disorder-scaling curves parametrized by the system sizes reveals a common intersection point at Δ_c. A similar feature of the distribution function of the IPR was found analytically for a critical ensemble of power-law random banded matrices in Refs. [20, 21]. This analogy allows us to interpret Δ_c as the critical point.

3 Numerical results

The LDT in the present model occurs at the top of the energy band (for $J > 0$). Therefore, to monitor the LDT only the uppermost eigenstate of the Hamiltonian (1) is considered hereafter. For doing this, we took advantage of the Lanczos method [22], enabling one to calculate a single eigenstate of the Hamiltonian (1), and computed the uppermost eigenstate for relatively large system sizes (up to about 6×10^4 sites). Open chains were used in all simulations.

Figure 1 demonstrates the driving effect of the exponent μ of the inter-site coupling on the character of the uppermost eigenstate. The simulations were performed for $\mu = 4/3 < 3/2$ and $\mu = 9/5 > 3/2$ and a moderate magnitude of disorder $\Delta = 5J$. The system size was set to $N = 2048$. As is seen, the eigenstates differ drastically from each other, spreading over the entire lattice for μ smaller than $3/2$, while being localized in the opposite case.

In Fig. 2 we show the results of a study of the disorder scaling of the ratio SDPN/MPN for different system sizes. The value $\mu = 4/3$ is chosen as an example. From this figure it follows that the relative PN fluctuation is indeed size-invariant at some value of the disorder magnitude; all curves plotted versus disorder have a joint intersection point. In this particular case, it is $\Delta_c = 10.2 \div 10.6\,J$ (slight size dependence of the intersection point is a finite size effect and is discussed below). This is the transition point. The figure demonstrate as well that both the MPN and the SDPN are of the same order of magnitude at the intersection for any system size, as was suggested in Refs. [20, 21] for the model of power-law random banded matrices. Remarkably, the disorder scaling of SDPN plotted separately shows a maximum in the vicinity of the transition (see Fig. 3), confirming the conjecture that the PN at transition is characterized by large fluctuations, the mean and the standard deviation of which of the same order of magnitude.

Contrary to the standard Anderson model with nearest-neighbor coupling, the contribution of long-range coupling terms to the spectrum of the Hamiltonian (1) converges very slowly upon increasing

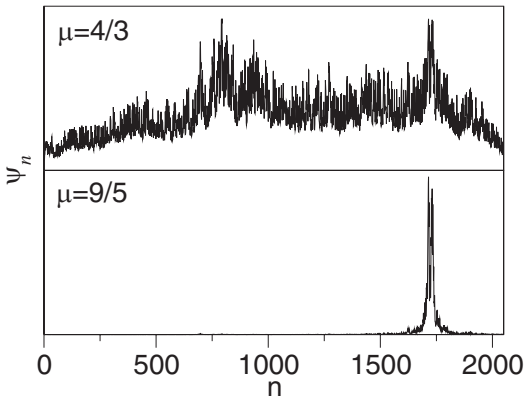

Fig. 1 Uppermost eigenstate for a) $\mu = 4/3$ and b) $\mu = 9/5$ and a moderate magnitude of disorder $\Delta = 5J$. The set of random site energies $\{\varepsilon_n\}$ is the same in both cases.

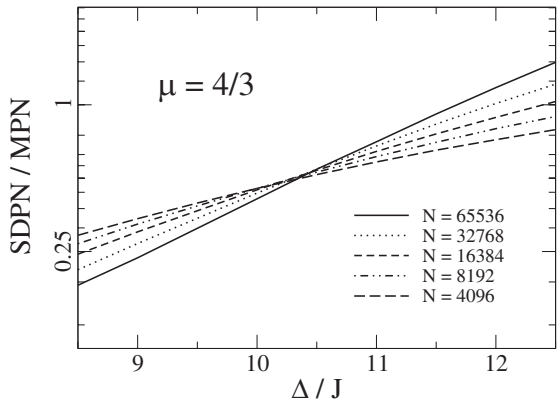

Fig. 2 Disorder scaling of the ratio SDPN/MPN for $\mu = 4/3$ in the vicinity of the joint intersection point at $\Delta = 10.2 \div 10.6\,J$. The curves are calculated for different system sizes N and averaged over more than $5 \times 10^3 \times (65536/N)$ disorder realizations.

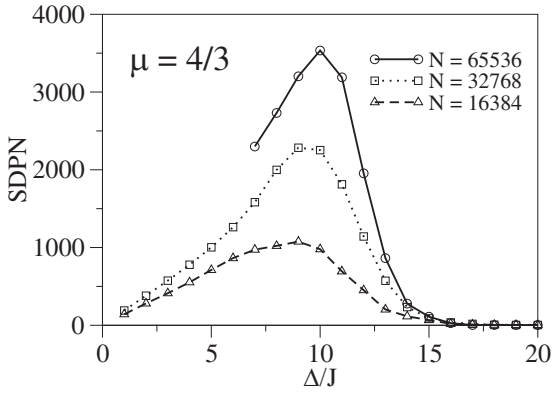

Fig. 3 SDPN of the uppermost state as a function of the degree of disorder Δ/J for $\mu = 4/3$ and different system sizes N. Notice the shift of the maximum to higher degree of disorder on increasing the system size.

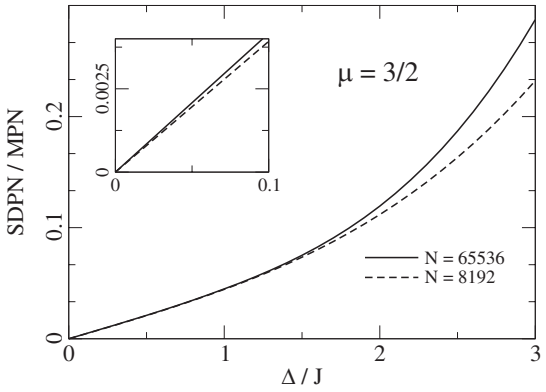

Fig. 4 Disorder scaling of the ratio SDPN/MPN for $\mu = 3/2$ in the vicinity of the joint intersection point at $\Delta_c = 0$. The curves are calculated for two different system sizes ($N = 8192$ and $N = 65536$) and averaged over more than 5×10^3 and 10^5 disorder realizations, respectively. The inset shows a blow up of the crossing point at the origin.

the system size. The convergence is dramatically slow for $\mu \to 1$. This results in a corresponding increase of the energy band width (actually, the upper band edge energy). Under cyclic boundary conditions the upper edge energy of the bare energy band depends on the system size N (at $N \gg 1$) as follows:

$$E(N) = 2\,\zeta(\mu) - \frac{C(\mu)}{N^{\mu-1}} + O\left(\frac{1}{N^{\mu}}\right) , \tag{3}$$

where $\zeta(\mu)$ is the Riemann ζ-function, $C(\mu) = 2\,\Gamma(2-\mu)\cos\left[\pi\,(\mu-1)/2\right]/(\mu-1)$, and $\Gamma(z)$ is the Γ-function. For an open chain, no analytical expression for the upper band edge $E(N)$ can be obtained. Nevertheless, its size scaling is close to Eq. (3) and the leading non-zero power of N in the expansion is also $1-\mu$. The increase of the energy band width with the system size means that disorder of the same magnitude is effectively stronger for smaller systems. This finite size effect introduces regular dependence of the critical disorder magnitude (that can be obtained by numerical analysis) on the system size. The contribution of other finite size effects, such as influence of boundary regions, can be expected to be weaker for larger systems due to very slow convergence of the upper band edge energy ($\propto N^{1-\mu}$). Our calculations of the relative PN fluctuation scaling confirm this conjecture. Accounting for the contribution of the the band edge size dependence, we obtained that the critical magnitude of disorder for $\mu = 4/3$ is $\Delta_c = (10.9 \pm 0.2)\,J$ in the thermodynamic limit ($N \to \infty$) [23].

Using the same technique we analyzed the localization properties of the model in the marginal case ($\mu = 3/2$), where the states are expected to be weakly localized [12]. Figure 4 shows the SDPN/MPN scaling curves of the uppermost state in the vicinity of the only joint intersection point that appears to be trivial: $\Delta_c = 0$. Thus, no signatures of the LDT are observed in the marginal case, indicating that all states are localized.

4 Conclusions

In summary, we demonstrated numerically that random Hamiltonians on 1D regular lattices with diagonal disorder and *non-random long-range* inter-site coupling, $J_{mn} = J/|m-n|^{\mu}$ ($J > 0$), revealed critical behavior at the top of the energy band provided $1 < \mu < 3/2$. To be specific, the system under-

goes a LDT on increasing the magnitude of disorder Δ. In order to prove this, we studied the disorder scaling of the ratio SDPN/MPN at different system sizes. We found that the ratio is a size-invariant parameter at some magnitude of disorder Δ_c, indicating the transition point. This finding suggests the usage of this invariance to monitor a LDT. In particular, for $\mu = 4/3$ the critical magnitude of disorder is at $\Delta_c = (10.9 \pm 0.2)\,J$ (in the thermodynamic limit). Thus, the one-parameter scaling theory of localization does not apply to this class of Hamiltonians.

In the marginal case ($\mu = 3/2$), the band edge states are expected to be weakly localized [12]. Studying the disorder scaling of SDPN/MPN for $\mu = 3/2$, we found that the critical point is trivial: $\Delta_c = 0$, which indicates that all states are localized in the marginal case at whatever finite disorder. To the best of our knowledge, this is the first direct numerical proof of state localization in the weak localization limit, without using the single-parameter scaling hypothesis.

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