To the possibility of a mobility edge in a random 1D lattice with long-range correlated disorder

Kozlov G.G.

March 4, 2014

Abstract

Tight-binding 1D random system with long-range correlations is studied numerically using the localisation criterium, which represents the number of sites, covered by the wave function. At low degrees of disorder the signs of a mobility edge, predicted in [2], were found. The possibility of exact mobility edge in the system under consideration is discussed.

Introduction

Absence of a mobility edge in 1D disordered systems with short-range correlations is well established [1]. Despite the fact that this statement is proved only for short-range correlated systems, the occurrence of a mobility edge in 1D random system with some particular long-range correlated disorder, reported in [2], seems to be very interesting and unexpected. The authors of [2] have managed to construct the correlated random potential for which the inverse localisation length (calculated theoretically for small degrees of disorder) was found to be zero for the central half-band of the energy spectrum and to be a non-zero constant for the remaining half-band. From the author’s of this note point of view, the infiniteness of localisation length is not an unambiguous criterium of localisation. For example, the zero-state in 1D chain with off-diagonal disorder has infinite localisation length [3] but, nevertheless, zero-state was found to be localised in sense of the basic Anderson criterium of localisation [4]. Therefore the verification of the result obtained in [2] by means of Anderson (or equivalent) criterium of localisation is necessary. The main task of this note is to put forward the additional arguments in favor of presence of a mobility edge in correlated 1D random chain, constructed by recipe [2]. To do this we perform the numerical exploration of eigen vectors of the random matrix of an appropriate disordered Hamiltonian by means of a criterium of localisation, differing from the finiteness of the localisation length.
1 1D long-range correlated random chain: the Hamiltonian.

The matrix of the Hamiltonian we are going to study has the tight-binding form

\[ H_{rr'} = \delta_{rr'} \varepsilon_r + \delta_{r,r+1} + \delta_{r,r-1}, \quad r, r', = 1, 2, ..., N \]  

(1)

with long-range correlated random potential \( \varepsilon_r \), generated in accordance with the following algorithm [2]:

\[ \varepsilon_r = \sum_{m=-\infty}^{\infty} G(r-m) \xi_m \quad G(m) = \sqrt{\frac{2}{3}} \frac{3}{2\pi m} \sin \left( \frac{2\pi m}{3} \right) \]  

(2)

where \( \xi_m \) are similarly distributed independent random numbers with \( \langle \xi_m \rangle = 0 \) and \( \langle \xi_m^2 \rangle = d^2/2 \) for any integer \( m \in [-\infty, +\infty] \). The degree of disorder is controlled by \( d \). As it was shown in [2], the spectral dependence of the inverse localisation length calculated for the Hamiltonian (1) with random potential (2) at small degree of disorder \( d \), goes down to zero in the central half-band \( E \in [-1, 1] \) and remains constant at \( E \in [\pm 2, \pm 1] \). The authors of [2] have interpreted this as the occurrence of a mobility edges at \( E = \pm 1 \). Below we verify this statement from the view point of our criterium of localisation, which is equivalent to the Anderson’s criterium.

2 Number of sites covered by the wave function: the criterium of localisation

We will start from reminding of a simple criterium of localisation, suggested in [4], which we will use below. We will characterise an arbitrary state \( \Psi \) by a number \( N^* \) of sites, covered by an appropriate wave function \( \Psi \), calculated as follows.

As \( \Psi \) is the eigen vector of a random Hamiltonian matrix in site representation, \( \Psi \) represents a vector-column with components \( \Psi_1, ..., \Psi_i, ..., \Psi_N \) where \( i \) is the site index. If \( |\Psi_i|^2 = 0 \) at a certain site \( i \), then this site is not covered by a state \( \Psi \) and is not taken into account while calculating \( N^* \). Vice versa, if \( |\Psi_i|^2 \) reaches its maximum \( |\Psi_i|^2 \) at the site \( i \), then this site is covered completely and its contribution while calculating \( N^* \) is equal to unit. In the general case, the contribution of an arbitrary site \( i \) is equal to \( |\Psi_i|^2 / |\Psi_i|^2 \) and we obtain the following formula for \( N^* \):

\[ N^* = N^*\{\Psi\} = \sum_{i=1}^{N} \frac{|\Psi_i|^2}{|\Psi_i|^2_{\text{max}}} = \frac{1}{|\Psi|^2_{\text{max}}} \]  

(3)

We can now introduce energy depending \( N^*(E) \) as follows. Let us specify some energy interval \( dE \ll E_{\text{max}} - E_{\text{min}} \) where \( E_{\text{max}} - E_{\text{min}} \) is a typical range of eigen energies for the random Hamiltonian under consideration. Consider all states with energies within the interval \( [E, E + dE] \) and denote by \( \sum_{E, E + dE} \) the summation over all these states. Now calculate \( N^*(E) \) as the following average value over all states with energies within the interval \( [E, E + dE] \):

\[ \langle N^*(E) \rangle = \frac{\sum_{E, E + dE} N^*(\Psi)}{\sum_{E, E + dE} 1} \]  

(4)
with \( \langle \rangle \) standing for the averaging over realisations of disorder. For small enough \( dE \) the function (4) does not depend on \( dE \). For the Hamiltonian represented by a random matrix of size \( N \), the function \( \langle N^*(E) \rangle \) in the spectral range of localised states should not depend on \( N \) (if \( N \) is large enough for \( \langle N^*(E) \rangle < N \) in this spectral region). In the spectral range of delocalised states (if it is exist), the function \( \langle N^*(E) \rangle \) must increase as \( \sim N \). This property of \( \langle N^*(E) \rangle \) one can use as a criterium for selection of localised and delocalised states in numerical experiments.

3 Results

In our calculations the auxiliary random values \( \xi_m \) were of gauss type with the distribution function in the form

\[
\rho(\xi) = \frac{1}{\sqrt{\pi d}} e^{-\frac{\xi^2}{d}}
\]

The spectral dependences of \( \langle N^*(E) \rangle \) for various sizes \( N = 1000, \ldots, 4000 \) of a random Hamiltonian matrix (1) at various degrees of disorder \( d = 0.1, 0.2, 0.4 \) are presented at Fig.1. From Fig.1 one can see that, at small disorder \( d = 0.1 \), the well-pronounced signs of delocalised states in the central half-band \( E \in [-1, 1] \) are observed. In this spectral range the number \( \langle N^*(E) \rangle \) of sites covered by the wave functions is proportional to the size \( N \) of a random matrix (1). At \( E \in [\pm 1, \pm 2] \) the number \( \langle N^*(E) \rangle \) does not depend on \( N \). As it was mentioned above, such a behaviour corresponds to the localised character of states at \( E \in [\pm 1, \pm 2] \). So, the signs of a mobility edge at \( E = \pm 1 \), predicted in [2], are observed.

Despite the fact that the above data have confirmed the statements of [2] there are at least two questions remain to be answered. The first question can be formulated as follows. In accordance with [2] the localisation length \( L_{\text{loc}} \) of states with energies in the range \( E \in [\pm 1, \pm 2] \) must be constant. But our calculations show that the number of sites \( \langle N^*(E) \rangle \) covered by the localised wave functions is strongly depend on energy in this energy interval (Fig.1b), varying from 7 – 8 (nearly zero) at \( E = \pm 1 \), varying from 7 – 8 (nearly zero) at \( E = \pm 2 \) to \( \sim 200 \) at the "mobility edge" \( E = \pm 1 \). It seems strange because both these quantities (\( \langle N^*(E) \rangle \) and \( L_{\text{loc}} \)) must describe the size of localised states and their energy dependance must be similar \( L_{\text{loc}} \sim \langle N^*(E) \rangle \). In our opinion this inconsistency reveals the ambiguous and disputable character of the localisation length as a measure of localisation of states.

The second question relates to the behaviour of the above random model at large degrees of disorder. The existence of a mobility edge (in the sense of inverse localisation length) was obtained in [2] in the limit of small disorder \( d \rightarrow 0 \). Whether it is possible to extend this result for the case of an arbitrary strong disorder? To clear up this we have studied the behaviour of \( \langle N^*(E) \rangle \) at large degrees of disorder. The results are presented at Fig.1(b,c). One can see that Fig.1(b,c) give grounds to conclude that at large disorder all states of the system are localised: the number of covered sites \( \langle N^*(E) \rangle \) for the states at the center of the band saturate, i.e. the nearly linear dependence \( \langle N^*(E) \rangle \) on \( N \), which takes place for \( d = 0.1 \) (Fig.1b), violates. Having this in mind, one can suppose that if we had an opportunity to make calculations for \( d = 0.1 \) (Fig.1a) with matrixes of the size greater than 4000, we would also observe the saturation of linear dependence of \( \langle N^*(E) \rangle \) on \( N \). Or there is some critical degree of disorder \( d_c \), such that for \( d > d_c \), the states in the center of the band become localised?
Figure 1: Panels (a), (b) and (c) – the spectral dependences of $\langle N^\ast(E) \rangle$ for various sizes $N = 1000, ..., 4000$ of a random Hamiltonian matrix (1) at various degrees of disorder $d = 0.1, 0.2, 0.4$. The matrix size $N$ and the degree of disorder $d$ are shown at the panels. In all cases the averaging over 100 realisations was performed, $dE = 0.012$. Panel (d) shows the realisation of a random potential (2).
In our opinion all these questions are still open.

Even if the further exploration of the correlated random system \([1], [2]\) will disprove the existence of exact mobility edge in this system, the curious spectral dependence of a number of covered sites \(\langle N^*(E) \rangle\) with a "mobility edge" (may be, virtual), looks very interesting.

References

[1] I. M. Lifshits, S. A. Gredeskul, and L. A. Pastur, Introduction to the Theory of Disordered Systems [in Russian], Nauka, Moscow (1982).

[2] F. M. Izrailev, A. A. Krokhin and N. M. Makarov, arXiv:1110.1762v1 [cond-mat.dis-nn]

[3] G. Theodorou, M. H. Cohen, Phys. Rev. B 13, 4597, (1976).

[4] G. G. Kozlov, arXiv:9909335 [cond-mat.dis-nn].