The generalized localization lengths in one dimensional systems with correlated disorder

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Abstract. The scale invariant properties of wave functions in finite samples of one dimensional random systems with correlated disorder are analyzed. The random dimer model and its generalizations are considered and the wave functions are compared. Generalized entropic localization lengths are introduced in order to characterize the states and compared with their behavior for exponential localization. An acceptable agreement is obtained, however, the exponential form seems to be an oversimplification in the presence of correlated disorder. According to our analysis in the case of the random dimer model and the two new models the possibility of power–law localization cannot be ruled out.

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1. Introduction

In a previous publication [1] we have introduced a new form of information length in order to characterize the shape of wave functions in finite one dimensional (1d) disordered systems. Using that definition we succeeded to show that the states in the 1d Anderson model with uncorrelated, onsite disorder do have, apart from oscillations, an overall exponential shape. Such an exponential decay has been found for practically any strength of disorder even in the case when the localization length exceeded the size of the system substantially.

The scaling properties of one–particle states in the presence of uncorrelated disorder in 1d and quasi–1d has been studied extensively both numerically and analytically [2, 3, 4, 5]. The similar problem of the more realistic case of correlated disorder has been recently considered in [6, 7]. In this paper we wish to present a scale invariant study on a wider family of correlated disorder in 1d and at the same time show how generalized localization lengths may help to analyze the properties of the one–particle eigenstates.

To be more specific the eigenvalue problem of an electron in a 1d disordered potential can be given as

\[ E c_m = \varepsilon_m c_m + V_{m,m+1} c_{m+1} + V_{m-1,m} c_{m-1} \]  

(1)

where \( c_m \) is the amplitude for the electron to be on site \( m \) and \( E \) is the energy eigenvalue. In the most simple case studied in [6] the onsite potentials \( \varepsilon_m \) are chosen randomly from a box distribution of width \( W \) centered around the origin, and the
off–diagonal hopping integrals are kept constant, $V_{m,m+1} = V_{m-1,m} = V_0$. The latter condition enables us to fix the unit of the energy scale $V_0 = 1$. For this model there are rigorous results \[8\] affirming complete exponential localization for any strength of disorder in infinite systems and in \[1\] we have proved numerically the above statement holds in finite systems, as well.

The effect of correlated disorder introduced in (1) has attracted much attention recently. These correlations maybe originated from interactions of electrons with lattice vibrations or, e.g., as a more realistic representation of disorder incorporating the presence of chemical bonding. The first models that included such correlations were therefore based on random binary models \[3, 10, 11, 12, 13, 14\]. These studies revealed the possibility that disorder correlations may increase and as well as decrease the localization length substantially.

In a special family of random binary alloys correlation was introduced by assigning the same energy level $\varepsilon_A$ or $\varepsilon_B$ to pairs of sites. This is called the random binary dimer model (RBDM). This model was first introduced in \[14\] and it has been shown that under certain conditions there are special $E_c$ values where the state is delocalized, transparent and the number of extended states around $E_c$ is proportional to the square root of the length of a finite sample. The localization length diverges at these energies \[3, 15\] and this is reflected in the conduction properties of finite samples \[16\]. In a recent paper \[7\] Izrailev et al. have studied the scaling properties of the eigenstates in the RBDM and succeeded to show that the states approaching $E_c$ are described similarly as in the case of uncorrelated disorder \[1, 3\].

There are other similar models formulated in the same spirit as the RBDM. A continuous Kronig–Penney type random dimer model \[17\] exhibits an infinite number of resonances with zero reflection constant. The existence of similar special states in a quasiperiodic dimer model has also been found in \[18\].

Exponential localization, although with an enhanced localization length has been seen in another model where the $\varepsilon_m$ energies are drawn from a box distribution but they are repeated for $L$ consecutive sites \[19\]. Here it is possible to vary $L$, however, no special energy with complete delocalization is present.

In this paper we present numerical results of two generalized versions (A, B) of the RBDM that are related to both the model of finite correlation length in \[19\] and the original model of Dunlap, Kundu and Phillips \[20\]. Our results are compared to the ones obtained by Izrailev et al. \[7\].

In Model A the onsite energies are drawn from a box distribution and assigned to two consecutive sites at the same time: it may be called general random dimer model (GRDM). This model is intermediate between the original Anderson model and the RBDM, it is in fact the special case of $L = 2$ of the model studied in \[19\]. As it has been shown \[19\] within such models the energy band does not contain any special energies where complete delocalization may occur, however, correlations change localization in a direction similar to the RBDM.

Model B \[20\] on the other hand contains disorder in both the diagonal and the off–diagonal part of (1)

\[
\begin{align*}
\varepsilon_m & = \frac{G}{\gamma}V_0(\alpha_{m,m+1} + \alpha_{m,m-1}) \\
V_{m,m\pm 1} & = V_0\sqrt{1 + \alpha_{m,m\pm 1}^2 - 2\alpha_{m,m\pm 1}\cos\delta}
\end{align*}
\]

(2)

where the quantities $\alpha_{m,m\pm 1}$ are chosen from a box distribution centered around the
origin with width \( W \leq 2 \). This model is obtained considering the coupling of electrons to the vibrations of the underlying lattice represented by the random variables \( \alpha_{m,m\pm 1} \) that introduce a correlated disorder in both the onsite and the off–diagonal matrix elements (see 2 for the details). The correlation is perfect if in (2) \( G = \gamma \). The RBDM can be considered as a simplified version of this model. The special energies where delocalization occurs are at \( E_c = 2V_0 \cos \delta \). We chose \( V_0 \) as the unit of energy here and varied the energy in the vicinity of \( E_c \) for different values of \( \delta \).

The solution of the Schrödinger equation (1) using appropriate initial conditions \( c_0 = c_1 = 1 \) is obtained by numerically iterating for a system of \( N = 10^4 \) sites and the localization properties of the eigenstates are calculated using the charge distribution \( Q_m = |c_m|^2 \). Averaging is performed over \( M = 1000 \) samples.

2. Shape analysis

The shape of the charge distribution \( Q_m \) may be characterized using the inverse participation number (IPN), \( D \), and the Shannon–entropy, \( H \)

\[
D^{-1} = \sum_m Q_m^2 \quad \text{and} \quad H = -\sum_m Q_m \ln Q_m. \tag{3}
\]

Both parameters \( D \) and \( \exp(H) \) give the number of sites effectively populated by the state. Therefore a state extending over the whole system would have \( D = N \) and \( H = \ln N \). This means that one may introduce two parameters \( \beta_1 \) and \( \beta_2 \)

\[
\beta_1 = \frac{1}{N} \exp(\overline{H} - H_{\text{ref}}) \quad \text{and} \quad \beta_2 = \overline{D}/D_{\text{ref}}, \tag{4}
\]

where normalization with respect to both the system size and the case of the absence of disorder has been performed. The latter is achieved by evaluating the values \( D_{\text{ref}} \) and \( H_{\text{ref}} \) for the Bloch–wave solution of (1) with \( \varepsilon_m = 0 \) and \( V_{m,m\pm 1} = V_0 \). Overbar means average over the samples at fixed energy and/or disorder. It is clear that both of these quantities change from 1 to 0 as disorder increases from 0 to \( \infty \) therefore in (6) they have been used as scaling functions.

Another way of expressing \( \beta_1 \) and \( \beta_2 \) can be obtained using our previous definitions (1). There we have used a size independent form and pointed out its relevance in a scale independent shape analysis of the states. In (3) we have calculated the spatial filling factor, \( q \), and the structural entropy, \( S \) of individual eigenstates as

\[
q = D/N \quad \text{and} \quad S_{\text{str}} = H - \ln D. \tag{5}
\]

These quantities obey the inequalities: \( 0 < q \leq 1 \) and \( 0 \leq S_{\text{str}} \leq -\ln q \). In the absence of disorder the solution of (1) is a plane wave for which \( q^0 = 2/3 \) and \( S^{0}_{\text{str}} = \ln 3 - 1 \). These quantities can be related to the reference values in (4) as \( q^0 = D_{\text{ref}}/N \) and \( S^0_{\text{str}} = H_{\text{ref}} - \ln D_{\text{ref}} \). Note that \( q^0 \) and \( S^0_{\text{str}} \) are independent of the system size while \( D_{\text{ref}} \) and \( H_{\text{ref}} \) are not. Using \( q \) and \( S_{\text{str}} \) we may rewrite equations (4) in the form

\[
\beta_1 = \overline{q} \exp(S_{\text{str}})/\beta_0 \quad \text{and} \quad \beta_2 = \overline{q}/q^0, \tag{6}
\]

where \( \beta_0 = q^0 \exp(S^0_{\text{str}}) \approx 0.7357 \). We have to note that the quantities \( q^0 \), \( S^0_{\text{str}} \) and \( \beta_0 \) that appear in (4) are obtained naturally from the solution of (1) for uncorrelated disorder which is a plane wave modulated by an exponentially decaying envelope represented as a product: \( c_m \sim \exp(-|m - m_0|/\xi) \sin(km + \delta) \)). The very same
conclusion was drawn using a completely different method by Fyodorov and Mirlin \[5\] based on results of quasi-1d systems and that of strictly 1d \[21\].

The main advantage of this reformulation is the application of the shape analysis proposed originally in \[22\]. We have shown in \[22\] and in other publications \[23, 24\] that our method is applicable for eigenstates composed as a product of several simple forms, e.g. an oscillating planewave and an envelope characterized by the scale \(\xi\). In \[23\] our method unambiguously showed the existence of power–law delocalized states near the mobility edge of a 1d quasiperiodic system, where both the bulk and the tail of the envelope played an equal role in the analysis of the wave functions.

It has been shown in \[22\] that parameters \(q\) and \(S_{str}\) can be calculated for ideal charge distributions analytically and that the relation \(S_{str}(q)\) is directly connected to the shape of the distribution. Therefore the properties of a large set of numerically obtained wave functions are compared to ideal curves in the parameter space \((q, S_{str})\) especially when some control parameters of the system are varied, e.g. system size, strength of disorder or energy. Similar relation may follow between \(\beta_1\) and \(\beta_2\). For example in the case of exponential localization we obtain

\[
\beta_1(z) = \frac{\exp(z) - 1}{z \exp(z) - 1} \exp \left(1 - \frac{z}{\exp(z) - 1}\right)
\]

(7)

and

\[
\beta_2(z) = \frac{2}{z} \left(1 - \frac{\exp(z) - 1}{\exp(z) + 1}\right)
\]

(8)

where \(z = N/\xi\) with localization length \(\xi.\) \(\beta_1(z)\) and \(\beta_2(z)\) are monotonous functions of \(z,\) hence the relation \(\beta_1 \rightarrow \beta_2\) exists and is also directly connected to the shape of the charge distribution. Note that similar analytic \(\beta_1(z)\) and \(\beta_2(z)\) functions can be calculated for any other type of form functions, e.g. for power–law decay.

3. Results and discussion

In \[7\] Izrailev et al. fitted a very simple analytic form for the relation \(\beta_1 \rightarrow \beta_2\) in the case of the RBDM

\[
\beta_2 = \frac{c\beta_1}{1 + (c - 1)\beta_1}
\]

(9)

with \(c \approx 0.5488.\) We will show that this relation is a good approximation, however, it fails to describe the states in both the localized and delocalized limits. We have to note that a similarly simple scaling relation \[3\] for the case of uncorrelated disorder has been exhaustively studied in \[5\] and shown the limitations of it.

In terms of \(q\) and \(S_{str}\) relation (9) reads as

\[
\tilde{S}_{str} = - \ln[c + (1 - c)\tilde{q}]
\]

(10)

where \(\tilde{S}_{str} = S_{str} - S_{str}^0\) and \(\tilde{q} = \beta_2 = \gamma_0/q^0.\) First of all in the most extended limit, \(\tilde{q} \rightarrow 1, S_{str}(\tilde{q}) \approx (1 - \tilde{q})/2\) should hold \[22\]. In contrast, according to (10) we get \(S_{str}(\tilde{q}) \approx (1 - c)/(1 - \tilde{q}).\)

Secondly we plotted the results of our calculations together with the data obtained from \[7\] in Figure 1. The analytical forms by equations (7,8) (solid curve) and also the empirical relation (9) (dotted curve) are shown, as well. It is clear that (9) is indeed a good approximation, however, the tendency is somewhat closer to equations (7,8)
Figure 1. Interrelation $\beta_2(\beta_1)$ of the generalized entropic lengths. Solid symbols are from [7], the crosses (DKPM) and open squares (GRDM) are results of the present calculation. The continuous curves stand for analytical relations. In the inset the difference $\Delta \beta = \beta_2 - \beta_1$ is given as a function of $\beta_1$. See details in the text.

that shows exponential localization on all length scales. The third relation (dashed curve) is the one derived assuming an envelope of the form $c_m \sim m^{-3}$ instead of an exponential form. The inset shows the deviation $\Delta \beta = \beta_2 - \beta_1$ as a function of $\beta_1$. In the inset we see again that relation (9) is an acceptable fit to the data from [7], however, in this figure it is very hard to check its accuracy especially for the localized and delocalized limits. In Figure 1 we have plotted our results for Models A and B, as well. For Model A we have varied the width of the box distribution between $W = 10^{-4}V_0$ up to $W = 10^4V_0$. In the case of Model B the parameters $W = 1.9V_0$ (here $W$ is limited to $0 \leq W < 2$) and $\delta = 0^\circ, 30^\circ, 60^\circ, 90^\circ$ have been used. We can see that, at least in terms of the $\beta_1 \to \beta_2$ relation, both of these models are not very much different from the behavior of RBDM.

In order to investigate the similarities and differences between the RBDM and the models studied here (Model A, the GRDM and Model B, the DKPM) it is even more apparent to plot $S_{str}$ as a function of $\ln q$. In Figure 2 the localized region $q \to 0$ is clearly not described by the relation (10) presented with a dotted line. It is also true that the states in neither models show clear exponential localization in the ideal form depicted by the continuous solid curve as it is already suggested in the previous paragraph. However, the states in Models A and B studied here are closer to it. This means that in the strong localization limit, $q \to 0$, the states in the RBDM have definitely more complex structure than that of Models A and B. It is interesting to note that similar deviation has been obtained for the case of weak uncorrelated disorder in [21]. However, in contrast to [21] our results are nonperturbative. Furthermore we have to stress that in the present work disorder correlations play an important role yielding the above mentioned deviations from conventional exponential localization.
The localization diagram for states in the RBDM, GRDM, and the DKPM. The relation \((10)\) \((\cdots \cdots)\) clearly deviates from the numerical results for \(q \rightarrow 0\). The symbols are like in Figure 1. In the inset the deviation of \(S_{str}\) is given from its expected universal form \((1 - q)/2\) when \(q \rightarrow 1\). The dotted line is wrong in this limit, as well.

In Figure 2 we have also plotted the \(S_{str}(q)\) relation for power–law localization with different exponents. We observe that the RBDM is well described by an overall shape: \(c_m \sim m^{-3}\) (dashed line) while the GRDM and the DKPM are better described with \(c_m \sim m^{-6}\) (dashed–dotted line). Apparently this is in contradiction with analytical expressions of the Lyapunov exponent (inverse localization length) which goes as \(\gamma(E) \sim (E - E_c)^2\) around the special energies \(E_c\) \([6, 15]\), however, \(\gamma\) should vanish for the case of power–law localization \([23, 24]\). A possible resolution to this problem is already outlined in Section 2, e.g. an exponential decay superimposed by some kind of rapidly varying substructure can easily provide a shift from the curve corresponding to the exponential decay to power–law decay as it is seen in Figure 2. According to Figure 2 the relation \((10)\) is a wrong approximation especially for the strong localization limit. Moreover, in the inset of Figure 2 we see deviations for the delocalized limit, \(q \rightarrow 1\), as well.

4. Conclusions

We have performed a shape analysis of wave functions obtained in several one dimensional random models with correlated disorder. We have introduced a new definition for the generalized localization lengths based on the inverse participation number and the Shannon–entropy. We have applied the shape analysis introduced in \([22]\).

It has been shown that the localization properties of the states in the RBDM are described by \((9)\) only approximately. On the other hand equation \((10)\) shows a wrong
behavior for \( q \to 1 \). Large deviations are obtained in the localized limit \( \beta_2 \to 0 \). We have compared the data from [7] with our simulations on the GRDM (Model A) and the DKPM (Model B). The data show a clear deviation from simple exponential localization: the average localization properties of the states for the RBDM resemble that of a power–law shape \( c_m \sim m^{-3} \) and in the case of Models A and B that of a power–law shape \( c_m \sim m^{-6} \).

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