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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 analysed. 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 behaviour 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.

1. Introduction

In a previous publication [1] we 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 in showing that the states in the 1D Anderson model with uncorrelated, on-site 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 where 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 have been studied extensively both numerically and analytically [2–5]. 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 analyse 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

$$Ec_m = \varepsilon_m c_m + V_{m,m+1}c_{m+1} + V_{m-1,m}c_{m-1} \tag{1}$$

where c_m is the amplitude of the probability for the electron to be at site m and E is the energy eigenvalue. In the simplest case studied in [1], the on-site potentials ε_m are chosen randomly from a box distribution of width W centred 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 for *infinite* systems,

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and in [1] we have proved numerically that the above statement holds for *finite* systems, as well.

The effect of correlated disorder introduced in (1) has attracted much attention recently. These correlations may have originated from interactions of electrons with lattice vibrations or e.g. in 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 [9–14]. These studies revealed the possibility that disorder correlations may increase as well as decrease the localization length substantially.

For a special family of random binary alloys, correlation was introduced by assigning the same energy level, ε_A or ε_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 for which the state is delocalized and 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 [6, 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 in showing that the states approaching E_c are described similarly to 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 ε_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 for 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 given by Dunlap, Kundu and Phillips [20]. Our results are compared to the ones obtained by Izrailev *et al* [7].

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

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

$$\begin{aligned} \varepsilon_m &= \frac{G}{\gamma} V_0(\alpha_{m,m+1} + \alpha_{m,m-1}) \\ V_{m,m\pm1} &= V_0\sqrt{1 + \alpha_{m,m\pm1}^2 - 2\alpha_{m,m\pm1}\cos\delta} \end{aligned} \tag{2}$$

where the quantities $\alpha_{m,m\pm1}$ are chosen from a box distribution centred around the origin with width $W \leqslant 2$. This model is obtained by considering the coupling of electrons to the vibrations of the underlying lattice represented by the random variables $\alpha_{m,m\pm1}$ that introduce a correlated disorder in both the on-site and the off-diagonal matrix elements (see [20] 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 for which delocalization occurs are $E_c = 2V_0 \cos\delta$. We chose V_0 as the unit of energy here and varied the energy in the vicinity of E_c for different values of δ.

The solution of the Schrödinger equation (1), using the 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 [1]:

$$D^{-1} = \sum_m Q_m^2 \qquad \text{and} \qquad H = -\sum_m Q_m \ln Q_m. \tag{3}$$

Both of the 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 [7]

$$\beta_1 = \frac{1}{N}\exp(\bar{H} - H_{ref}) \qquad \text{and} \qquad \beta_2 = \bar{D}/D_{ref} \tag{4}$$

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_{ref} and H_{ref} for the Bloch-wave solution of (1) with $\varepsilon_m = 0$ and $V_{m,m\pm1} = V_0$ [7]. The overbar indicates averaging over the samples at fixed energy and/or disorder. It is clear that both of these quantities change from 1 to 0 as the disorder increases from 0 to ∞; therefore in [7] they have been used as scaling functions.

Another way of expressing β_1 and β_2 (equation (6) below) can be obtained using our previous definitions [1]. There, we used a size-independent form and pointed out its relevance in a scale-independent shape analysis of the states. In [1] we calculated the spatial filling factor, q, and the structural entropy, S_{str}, of the individual eigenstates as

$$q = D/N \qquad \text{and} \qquad S_{str} = H - \ln D. \tag{5}$$

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

$$\beta_1 = \bar{q}\exp(\bar{S}_{str})/\beta_0 \qquad \text{and} \qquad \beta_2 = \bar{q}/q^0 \tag{6}$$

where $\beta_0 = q^0\exp(S^0_{str}) \approx 0.7357$. We have to note that the quantities q^0, S^0_{str} and β_0 that appear in (6) 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: $c_m \sim \exp(-|m - m_0|/\xi)\sin(km + \delta)$ [1]. The very same conclusion was drawn using a completely different method by Fyodorov and Mirlin [5] on the basis of results for quasi-1D systems and for strictly 1D systems [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 products of several simple forms, e.g. an

oscillating plane wave and an envelope characterized by the scale ξ. In [23] our method unambiguously showed the existence of power-law delocalized states near the mobility edge of a 1D quasiperiodic system, where the bulk and the tail of the envelope played equal roles in the analysis of the wave functions.

It was shown in [22] that the parameters q and S_{str} can be calculated for ideal charge distributions analytically and that the function $S_{str}(q)$ is directly connected to the shape of the distribution. Therefore the properties of a large set of wave functions obtained numerically are to be 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 relations between β_1 and β_2 may follow. For example, in the case of exponential localization we obtain

$$\beta_1(z) = \frac{\exp(z) - 1}{z \exp(z)} \exp\left(1 - \frac{z}{\exp(z) - 1}\right) \tag{7}$$

and

$$\beta_2(z) = \frac{2}{z}\left(\frac{\exp z - 1}{\exp z + 1}\right) \tag{8}$$

where $z = N/\xi$ with ξ the localization length. $\beta_1(z)$ and $\beta_2(z)$ are monotonic functions of z, and hence there is a relation between β_1 and β_2 and it 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 function, e.g. for power-law decay.

3. Results and discussion

In [7] Izrailev *et al* fitted a very simple analytic form for the relation between β_1 and β_2 in the case of the RBDM:

$$\beta_2 = \frac{c\beta_1}{1 + (c - 1)\beta_1} \tag{9}$$

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 the limitations of it shown.

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

$$\tilde{S}_{str} = -\ln[c + (1 - c)\tilde{q}] \tag{10}$$

where $\tilde{S}_{str} = \bar{S}_{str} - S^0_{str}$ and $\tilde{q} = \beta_2 = \bar{q}/q^0$.

First of all, in the most extended limit, $\tilde{q} \to 1$, $\tilde{S}_{str}(\tilde{q}) \approx (1 - \tilde{q})/2$ should hold [22]. In contrast, according to (10) we get $\tilde{S}_{str}(\tilde{q}) \approx (1 - c)(1 - \tilde{q})$.

Secondly, we plotted the results of our calculations together with the data obtained from [7] in figure 1. The analytical forms obtained from equations (7) and (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) and (8), which shows exponential localization on all length scales. The third relation (the 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 β_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

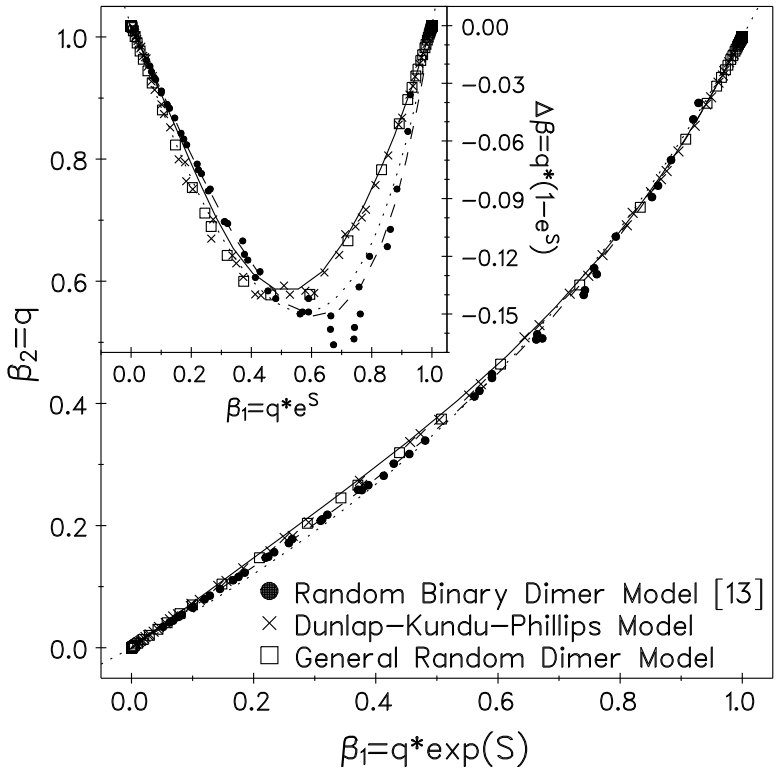

Figure 1. The interrelation of β_2 and β_1 for the generalized entropic lengths. The solid symbols are from [7], while the crosses (DKPM) and open squares (GRDM) represent results from the present calculation. The continuous curves represent analytical relations. In the inset, the difference $\Delta\beta = \beta_2 - \beta_1$ is given as a function of β_1. See the details in the text.

we have varied the width of the box distribution between $W = 10^{-4}V_0$ and $W = 10^4 V_0$. In the case of model B the parameters $W = 1.9V_0$ (here W is limited to $0 \leqslant W < 2$) and $\delta = 0^\circ, 30^\circ, 60^\circ, 90^\circ$ have been used. We can see that, at least in terms of the relation connecting β_1 and β_2, neither of these models is very different from the behaviour of the RBDM.

In order to investigate the similarities of and differences between the RBDM and the models studied here (model A, the GRDM and model B, the DKPM), it is even more transparent 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) represented with a dotted line. It is also true that for neither model do the states show a clear exponential localization in the ideal form depicted by the continuous solid curve, as had been suggested in the previous paragraph. However, the states in models A and B studied here come closer to doing this. This means that in the strong-localization limit, $q \to 0$, the states in the RBDM definitely have more complex structure than those of models A and B. It is interesting to note that a similar deviation has been obtained for the case of weak uncorrelated disorder in [21]. However, in contrast to those given in [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.

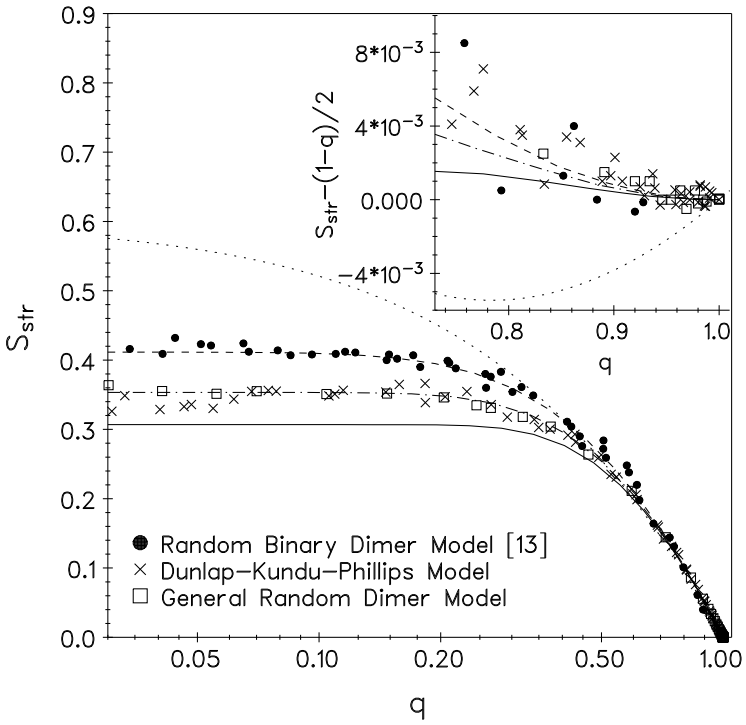

Figure 2. The localization diagram for states in the RBDM, the GRDM and the DKPM. Relation (10) (· · · · · ·) clearly deviates from the numerical results for $q \to 0$. The symbols are the same as for figure 1. In the inset the deviation of S_{str} from its expected universal form $(1-q)/2$ when $q \to 1$ is given. The dotted line is wrong in this limit, as well.

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

4. Conclusions

We have performed a shape analysis of the wave functions obtained from 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 incorrect behaviour 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 for 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* those of a power-law shape $c_m \sim m^{-3}$ and in the case of models A and B those of a power-law shape $c_m \sim m^{-6}$.

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