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LETTER TO THE EDITOR

A new self-consistent approximation for the mobility edge trajectories

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Abstract. A new approximation for mobility edge trajectories, previously proposed in analogy with the Bethe–Peierls approximation in magnetic systems, is analysed in detail. Mobility edge trajectories for several types of probability distribution of site energies on the three-dimensional cubic lattice are obtained. The present results agree qualitatively with those obtained by the finite-size scaling method.

A large number of studies has been made on the Anderson transition [1–5]. It is probably fair, however, to say that the critical phenomenon at the mobility edge has not yet been fully understood. For instance, little is known about the upper critical dimensionality. Hence it is still a challenging problem to study the localization transition to clarify its critical dimensionalities and the universality of the critical exponents.

It is important for study of the upper critical dimensionality to know the critical phenomena in high dimensions. In spin systems, it is well known that the Weiss mean-field approximation becomes exact in the limit of high dimensionality [6, 7]. In fermionic systems, on the other hand, such an approximation has not yet been established. Over the past few years, however, considerable progress has been made on strongly correlated fermionic systems in high dimensions [8–12]. A mean-field theory for the simplified Hubbard model based on the analysis on the Bethe lattice, which is often considered as an infinite dimensional lattice, has been obtained [9]. This progress suggests that, even in the case of the localization transition, critical phenomena in the Bethe lattice may be related, in some ways, to those in the regular lattice in high dimensions. In this context, we have proposed a possible approximation for the mobility edge (E_c) on the d-dimensional *hypercubic lattice* based on some exact results on the Bethe lattice [13]. It can be said that our approximation would correspond to the Bethe–Peierls approximation in spin systems. We have shown that our approximation for the mobility edge works well in the case of the Lorentzian probability distribution of site energies [13]. However, this result may be due to some specific property of the Lorentzian distribution whose second moment, for instance, is infinite. It is important therefore to clarify whether or not our new formula works also for other types of probability distribution of site energies. We have carried out, in this paper, numerical calculations on the mobility edge trajectories, using our formula, for two types of probability distribution of site energies, namely, the Gaussian and the box distributions. Notice that their second moments are both finite. We have found that our approximation also yields qualitatively reasonable results for these two cases.

We consider the tight-binding Anderson model defined by the Hamiltonian

$$H = -t \sum_{(i,j)} C_i^\dagger C_j + \sum_i V_i C_i^\dagger C_i \tag{1}$$

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where $C_i^\dagger$ (C_i) is a creation (annihilation) operator of an electron at the site i. The site energies $\{V_i\}$ are distributed independently with the distribution function $P(V)$. In our previous paper [13], we show that the decay rate λ_E of the Green function on the Bethe lattice defined by

$$\lambda_E \equiv -\lim_{|i-j|\to\infty} \frac{1}{|i-j|} \ln|G(i, j; E)| \tag{2}$$

is given by

$$\lambda_E = \int Q(y) \ln|y| \mathrm{d}y - \ln|t| \tag{3}$$

with the solution $Q(y)$ of the non-linear integral equation

$$Q(y) = \int P\Big(E - y - t^2 \sum_{l=1}^{K} y_l^{-1}\Big) \prod_{l=1}^{K} Q(y_l)\mathrm{d}y_l. \tag{4}$$

Here K is the connectivity of the Bethe lattice and $G(i, j; E)$ denotes the Green function between the site i and the site j at energy $E \in \boldsymbol{R}$ on the Bethe lattice, which is assumed to be sufficiently large but finite. Although our analysis in the previous paper [13] was restricted to the case of the Lorentzian distribution of site energies, we expect that the above formula also holds for the box and the Gaussian distributions of site energies.

Our criterion for the mobility edge (E_c) on the d-dimensional *hypercubic lattice* is then given by the condition that [13]

$$\lambda_E - \ln K = 0 \tag{5}$$

with $K = (2d - 1)$. In our approximation, therefore, the mobility edge E_c can be obtained by solving the non-linear integral equation (4) with $K = (2d - 1)$ and by evaluating the integral (3). Physically, the function $Q(y)$ denotes the distribution of a Green function defined by a modified Hamiltonian on the Bethe lattice, and hence it is a non-negative function [13]. For the Lorentzian distribution of site energies defined by

$$P(V) = \frac{1}{\pi} \frac{\gamma}{V^2 + \gamma^2} \tag{6}$$

the non-linear equation (4) can be solved analytically and the condition (5) reduces to [13]

$$\frac{E^2}{(2d)^2} + \frac{\gamma^2}{(2d-2)^2} = t^2 \tag{7}$$

The mobility edge in this case is therefore given by an elliptic curve and, as shown in the previous paper [13], our result is quite consistent with that obtained by Bulka *et al* [13, 14]. In the case of the Gaussian and the box distributions, on the other hand, we have to solve the non-linear equation (4) numerically.

To obtain the distribution $Q(y)$ numerically, we have adopted a Monte Carlo method. Let us consider the three-dimensional case where $2d - 1 = 5$. First, we generate $N = 5^9$ samples $\{y_i; i = 1, \ldots, N\}$ as an initial set of values of y. We carry out the following procedure to generate a new set $\{y_i'; i = 1, \ldots, N\}$. For each i ($i = 1, \ldots, N$), we choose at random $2d-1=5$ values $(x_1^{(i)},\ldots,x_5^{(i)})$ of y from the set $\{y_i\}$ and also generate a random variable V_i according to the distribution $P(V)$. Then we generate the new set $\{y_i'\}$ using the relations

$$y_i' = E - V_i - t^2\sum_{j=1}^{5}(x_j^{(i)})^{-1} \qquad i=1,\ldots,N. \tag{8}$$

By repeating this procedure, we can obtain the distribution function $Q(y)$ and thus we can estimate numerically the expectation value $\langle\ln|y|\rangle \equiv \int \ln|y|Q(y)\,dy$ in the right-hand side of (3) for fixed energy E and the given probability distribution $P(V)$ of site energies. Strictly speaking, the new samples $\{y_i'; i=1,\ldots,N\}$ generated from the set $\{y_i; i=1,\ldots,N\}$ are not completely independent. To see whether or not this fact causes systematic errors in our calculations, we have performed these procedures for the Lorentzian distribution of site energies for which the exact value of $\langle\ln|y|\rangle$ has already been obtained analytically [13]. The above procedure is carried out up to 500 iterations and in this range we have observed no systematic deviation from the exact value (figure 1). We have also checked for the box distribution that no systematic increase or decrease of the expectation value has been observed within the same number of iterations. From these results, it seems reasonable to suppose that the true expectation value can be correctly estimated by these procedures. Let us denote the distribution $\{y_i^{(m)}; i=1,\ldots,N\}$ after m iterations by $Q_m(y)$ and the expectation value of $\ln|y|$ for Q_m by $\langle\ln|y|\rangle_m \equiv \sum_i \ln|y_i^{(m)}|/N$. We have found that Q_m approaches Q quite rapidly. After 30 or 40 iterations, the distribution Q_m can be regarded to have already converged on the steady solution Q. We have thus used the expectation values $\{\langle\ln|y|\rangle_m; m=60,\ldots,120\}$ to estimate the true expectation value $\langle\ln|y|\rangle$. From the condition (5), the mobility edges for the Gaussian and the box distributions are then obtained as shown in figure 2 and figure 3, respectively. The Gaussian and the box distributions we have used are given by

$$P_G(V) = \left(\frac{6}{\pi W_G^2}\right)^{1/2}\exp\left(-\frac{6V^2}{W_G^2}\right) \tag{9}$$

and

$$P_B(V) = \frac{1}{W_B}\theta(W_B/2-|V|) \tag{10}$$

respectively. The second moments of P_G and P_B coincide with each other if $W_G = W_B$.

As shown in figures 2 and 3, in the cases of the Gaussian and the box distributions we have extended states not only inside the unperturbed band ($|E|<6|t|$), but also outside the unperturbed band ($|E|>6|t|$). This is in contrast with the case of the Lorentzian distribution of site energies, in which case the extended states do not exist outside the unperturbed band (figure 4) [13]. All these qualitative features for the mobility edge trajectories agree with those obtained by the finite-size scaling method [14]. The present approximation thus seems to work well not only for the Lorentzian distribution but also for other types of distribution whose second moments are finite. For the box and the Gaussian distributions, the critical values of the width of the distribution of site energies at the centre of the band ($E=0$) are estimated as $W_B^c/t = 25.24\pm0.08$ and $W_G^c/t = 29.64\pm0.10$, respectively. These values are slightly larger than those obtained by other methods [14, 15]. For instance, the values obtained by Bulka *et al* [14] are $W_B^c/t = 16.3\pm0.5$ and $W_G^c/t = 20.9\pm0.5$. Numerical

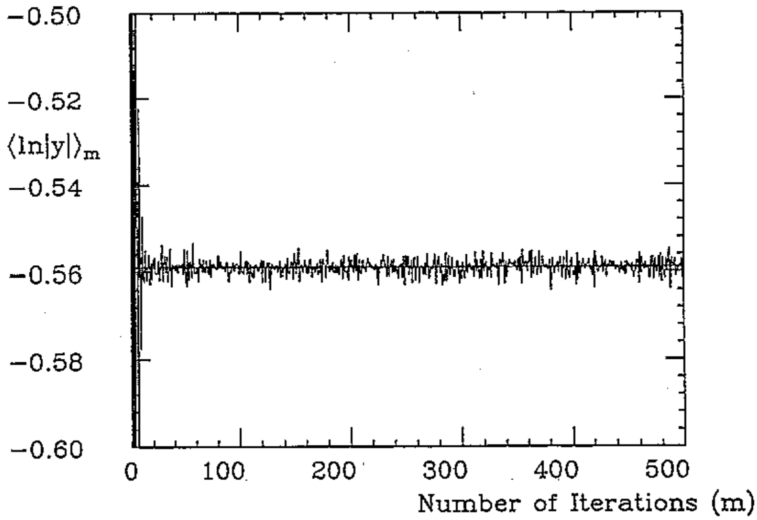

Figure 1. Convergence of $\langle \ln|y| \rangle_m$ when the procedure is iteratively carried out in the case of the Lorentzian distribution of site energies with $\gamma = 1$ and $E = 2$. The horizontal axis represents the number of iterations (m) and the exact expectation value $\langle \ln|y| \rangle = -0.5589932\ldots$ is represented by the horizontal line.

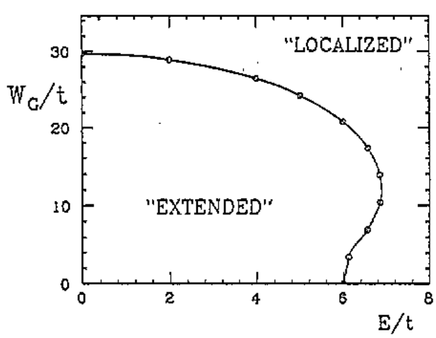

Figure 2. The mobility edge trajectory obtained by the present approximation for the Gaussian distribution of site energies on the three-dimensional hypercubic lattice. The critical value of the width of the distribution at $E = 0$ is estimated as $W_G^c/t = 29.64 \pm 0.10$.

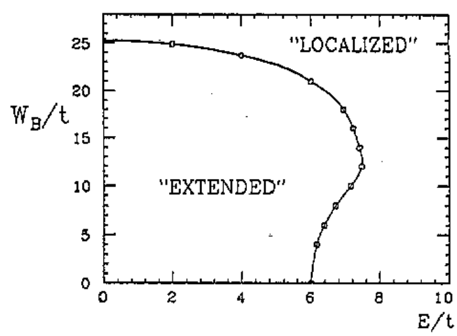

Figure 3. The mobility edge trajectory obtained by the present approximation for the box distribution of site energies on the three-dimensional hypercubic lattice. The critical value of the width of the distribution at $E = 0$ is estimated as $W_B^c/t = 25.24 \pm 0.08$.

discrepancies may arise from the fact that interference effects are not taken into account in the present approximation and it is likely that this fact will enhance the extended states.

We also find that in the case of the Lorentzian distribution the above discrepancy between the result ($\gamma_c/t = 4$) obtained by the present approximation [13] and that ($\gamma_c/t = 3.8 \pm 0.5$) obtained by Bulka *et al* [14] is small compared with those in the cases of the Gaussian and the box distributions. This can be explained as follows. As already mentioned, the second moment for the Lorentzian distribution is infinite and therefore extremely high or low site energies will contribute more dominantly compared with the case of the other two types of distribution. It is then likely that in the case of the Lorentzian distribution transmissions and reflections at such extremely high or low site energies would become more important

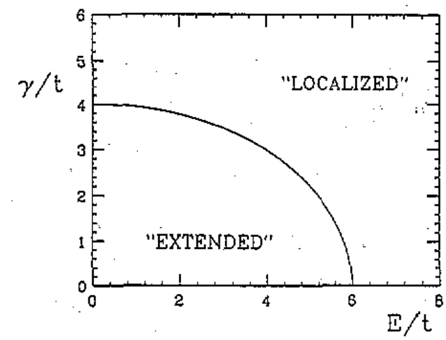

Figure 4. The mobility edge trajectory obtained by the present approximation for the Lorentzian distribution of site energies on the three-dimensional hypercubic lattice, which is taken from [13].

and, as a result, interference effects become less important accordingly. This would be the reason why the present approximation yields also a quantitatively reasonable result for the Lorentzian distribution of site energies.

In summary, we have numerically evaluated the mobility edge trajectories for the Gaussian and box distributions of site energies using a new approximation, which was proposed in analogy with the Bethe–Peierls approximation in magnetic systems. Together with the previous result (7) for the Lorentzian distribution of site energies [13], it is shown that the present approximation correctly describes the qualitative change of the mobility edge trajectories for these three types of probability distribution; both the re-entrant phenomena outside the unperturbed band for the Gaussian and box distributions and the absence of extended states outside the unperturbed band for the Lorentzian distribution [14–16] are indeed reproduced. Note that the criterion for localization in the previous work [17–19] does not reproduce the qualitative property of the mobility edge trajectory for the Lorentzian distribution of site energies [18]. We argued [13] that the effect of closed loops is neglected in the present approximation since it is based on the decay rate of the Green function on the Bethe lattice. Usually, it is thought that interferences due to closed loops are important in the Anderson transition. Hence it is rather remarkable that the present approximation for the mobility edge yields qualitatively reasonable results in three-dimensional systems. It is expected that this approximation would hold better in higher dimensions, where interference effects become less important. The relationship between localization itself on the Bethe lattice [17–22] and that in the limit of high dimensionality has already been discussed by several authors [22–25]. Whether or not the present approximation becomes exact in high dimensions remains to be seen.

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