Localization and phase coherence length in the Lloyd model

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The coefficient for exponential attenuation of the averaged Green function $[\lim_{\delta\to 0}\langle G_{\mathbf{OR}}(E+i\delta)\rangle_{\mathrm{av}}\sim e^{-\kappa R}]$ is calculated for several infinite lattices in one, two, and three dimensions with a diagonal Lorentzian disorder of site energies (Lloyd model). In the limit of extended states, $l=\kappa^{-1}$ coincidences with the phase coherence length and with the mean free path associated with $|\mathbf{k}\rangle$ states. In the opposite limit, that of strongly localized states, the inequality $\kappa\geq\gamma$ is almost satisfied as an equality where γ is the inverse localization length. Our results for κ are the same as those calculated by Johnston and Kunz who associate their results with γ, that is, with the localization length. This leads us to reinterpret their results and to conclude that, when the dimensionality is higher than 2, there is still a strong possibility of a mobility edge in this model.

INTRODUCTION

Tight-binding Hamiltonians of the form

$$\hat{\mathscr{H}}=\sum_{\mathbf{R}}\varepsilon_{\mathbf{R}}|\mathbf{R}\rangle\langle\mathbf{R}|+\sum_{\mathbf{R},\Delta\mathbf{R}}V|\mathbf{R}\rangle\langle\mathbf{R}+\Delta\mathbf{R}|\ , \tag{1}$$

with a Lorentzian distribution of site energies $P(\varepsilon)=\pi^{-1}\Gamma/(\varepsilon^2+\Gamma^2)$ have been intensively studied since their introduction by Lloyd,[1] due to the simplicity in finding various averages. However, conclusions as to the localization of states in this model have been extensively variable.[1-6] After the original statement of Lloyd that all states would be extended here, regardless of dimensionality, other authors predicted a mobility edge[2] using the $L(E)$ method. Finally, quite recently Johnston and Kunz[6] (hereafter JK) find that all states are localized, independently of the dimensionality d. Even when this result is in agreement with the predictions of the scaling theory of localization for the case of $d=1$ and $d=2$, for higher d it does not provide the expected mobility edges.

Localization of states is characterized by the inverse localization length $\gamma(E)$. As has been shown, $\gamma(E)$ gives the smallest Lyapunov characteristic exponent for the growth of the product of random transfer matrices.[6] This exponent also describes the asymptotic exponential decay of $G_{0,\mathbf{R}}(E)=\langle\mathbf{0}|(E\hat{\mathbf{1}}-\hat{\mathscr{H}})^{-1}|\mathbf{R}\rangle$ as $R\to\infty$,[7,8] and it is usually defined as

$$\gamma(E)=\lim_{R\to\infty}\left[-\frac{1}{R}\lim_{\delta\to 0}\ln|G_{0,\mathbf{R}}(z)|\right], \tag{2}$$

where $z=E+i\delta$ with $\delta\geq 0$. It must be noted that the dispersion of the term in parentheses, for different members of an ensemble, tends to zero as $R\to\infty$. Thus $\gamma(E)$ is a self-averaging magnitude. Then, different forms of averaging of this term gives the same result.

Even when analytical expressions for $\gamma(E)$ are difficult to find in the general case, a reliable expression for $\gamma(E)$ has been given for Lorentzian disorder in one dimension.[3,5] Recent results for higher dimensions[6] are controversial and will be discussed further ahead.

In this work we study the function $\kappa(E)$ defined by

$$\kappa(E)=\lim_{R\to\infty}\left[-\frac{1}{R}\ln|\lim_{\delta\to 0}\langle G_{0,\mathbf{R}}(z)\rangle_{\mathrm{av}}|\right]. \tag{3}$$

Due to its definition, $\kappa(E)$ does not directly describe localization. This is because not only the localization of states, but also the phase incoherence of $G_{0,\mathbf{R}}(E)$ for different members of the ensemble, contribute to $\kappa(E)$. Mathematically it can be shown that there is an inequality between $\gamma(E)$ and $\kappa(E)$, because their definitions are similar except by the nontrivial order of taking the average, the limit $\delta\to 0$, and the magnitude of $G_{0,\mathbf{R}}$. In the general case one has a relation between a mean of the self-averaging magnitude given in (2) and $\kappa(E)$:

$$\gamma(E)\leq\kappa(E)\ , \tag{4}$$

which follows from the Schwartz inequality.

The usefulness of the expressions for $\kappa(E)$ arises because it has a clear physical meaning for very weak disorder and very strong disorder. In the limit of weak disorder, $l(E)=\kappa^{-1}(E)$ is the length over which the phase coherence of $G_{0,\mathbf{R}}$ is maintained. Then, closed expressions for $\kappa(E)$ can be used to heuristically associate a value of Γ to a system with the mean free path of a weak disordered system. This is also the length at which (according to Anderson *et al.*,[9]) one should begin to see universality in the scaling process. In the opposite limit of strong disorder, one has a near equality $\gamma(E)\simeq\kappa(E)$ for strongly localized states; thus in calculating κ, one obtains an approximate expression for γ. These properties make it worthwhile to obtain exact expressions for $\kappa(E)$ and compare them with known results for the inverse localization length for this model.

JK have calculated the Lyapunov characteristic exponent for d-dimensional hypercubic systems of finite transverse cross section with Lorentzian disorder. In the limit of infinite cross section, they found analytical expressions in which the localization length (γ^{-1}) is always

finite. In this limit, γ was found to be independent of both the dimensionality and the energy, for $|E|<2(d-1)|V|$. Based on these calculations, JK tentatively conclude that all states would be localized in any d-dimensional system with Lorentzian disorder. These results appear to disqualify the Lorentzian disorder as a physically sensible model for a disordered system. However, their results rest on the definition they used for the mean of $\gamma(E)$, since they assumed that this mean can be obtained as an analytical continuation from the complex plane. Moreover, as we shall show below, their results for $\gamma(E)$ coincide with $\kappa(E)$ defined by (3). We will show that this is due to their starting assumptions, which is misleading because of the different order in taking the ensemble average and the limit $\delta\to 0$, which are not equivalent.

RESULTS

Our strategy will be to obtain $\kappa(E)$ directly for infinite lattices, instead of considering finite cross section. Following Lloyd,[1] one can write the averaged Green's function as

$$\lim_{\delta\to 0}\langle G_{0,\mathbf{R}}(E+i\delta)\rangle_{\mathrm{av}}=G^0_{0,\mathbf{R}}(E+i\Gamma)=\frac{1}{(2\pi)^{d-1}}\int d\mathbf{k}_{||}\,\tilde{G}^{\,0}_{0,x}(\mathbf{k}_{||},E+i\Gamma)\times e^{i\mathbf{k}_{||}\cdot\mathbf{R}_{||}} \tag{5}$$

with $\mathbf{R}=(x,\mathbf{R}_{||})$ where $G^0_{0,\mathbf{R}}$ is the resolvent for the ordered system ($\Gamma=0$) evaluated on the complex plane. $\tilde{G}^{\,0}_{0,x}(\mathbf{k}_{||},E+i\Gamma)$ is the resolvent for the ordered one-dimensional system with site and hopping energies renormalized as follows:

$$\tilde{\varepsilon}_0=\sum_{\substack{\mathbf{R}'_{||}\\ x'\equiv 0}} e^{i\mathbf{k}_{||}\cdot\mathbf{R}'_{||}}V_{0,\mathbf{R}'}\ ,$$

$$\tilde{V}_{0,x}=\sum_{\substack{\mathbf{R}'_{||}\\ x'=x}} e^{i\mathbf{k}_{||}\cdot\mathbf{R}'_{||}}V_{0,\mathbf{R}'}\ .$$

In the special case of finite cross section, the integral over $\mathbf{k}_{||}$ reduces to a sum. By inspection of Eq. (5) one can see that it is a generalization to an arbitrary lattice of Eq. (3.11) of JK. This means that their assumptions lead them to an expression for $\gamma(E)$ that is the same as the one we found for $\kappa(E)$. On the other hand, each $\tilde{G}^{\,0}_{0,x}$ decays exponentially as $x\to\infty$ with a coefficient that depends on $\mathbf{k}_{||}$. For systems of finite cross section, $\kappa(E)$ coincides with the smallest of these coefficients. However, in the case of infinite cross section the interferences in the integral over $\mathbf{k}_{||}$ could lead *a prior* to a κ different from this minimum.

In what follows, we give the results of the evaluation of (5) for systems which are infinite in all their spatial dimensions.

Case (a). For the linear chain,

$$\kappa=\cosh^{-1}\left\{\left[\left[\frac{E-E_S}{E_S-E_I}\right]^2+\left[\frac{\Gamma}{E_S-E_I}\right]^2\right]^{1/2}+\left[\left[\frac{E-E_I}{E_S-E_I}\right]^2+\left[\frac{\Gamma}{E_S-E_I}\right]^2\right]^{1/2}\right\}, \tag{6}$$

where κ is in units of inverse distance between nearest-neighbor atoms. $E_S=2V$ and $E_I=-2V$ are the top and bottom band edges of the ordered system. In Fig. 1 we show the graph for $l(E)=\kappa^{-1}(E)$,

Case (b). For the square lattice [with $\mathbf{R}$ in the (1,1) direction]

$$\kappa=\cosh^{-1}\left[\left\{\left[\left[\frac{E}{2V}\right]^2-\left[\frac{\Gamma}{2V}\right]^2\right]^2+\left[\frac{E\Gamma}{8V^2}\right]^2\right\}^{1/2}+\left\{\left[1+\left[\frac{\Gamma}{4V}\right]^2-\left[\frac{E}{4V}\right]^2\right]^2+\left[\frac{E\Gamma}{8V^2}\right]^2\right\}^{1/2}\right]. \tag{7}$$

Here $\kappa^{-1}(E)$ is shown in Fig. 2 for different values of disorder.

Case (c). For a square lattice with $V/2$ interactions to second-nearest neighbors [$\mathbf{R}$ is in the (1,0) direction] κ is obtained from Eq. (6) with $E_S=6V$ and $E_I=-2V$, which are the position of the band edges for the $\Gamma=0$ system. We omit a graph for this case or the following cases since they coincide with that of Fig. 1 with appropriate changes of scale for E and Γ. One sees that $\kappa^{-1}(E)$ does not show any special feature for $E\simeq -2V$, where the density of states diverges logarithmically for $\Gamma=0$.

Case (d). For a bcc lattice [$\mathbf{R}$ in the (1,0,0) direction], κ has an expression analogous to (6), with $E_S=8V$, $E_I=-8V$, which are the band edges of the ordered systems.

Case (e). For a fcc lattice [$\mathbf{R}$ in the (1,0,0) direction], again, κ has the form (6) with $E_S=12V$ and $E_I=-4V$. One notes that except for an energy shift, $l(E)$ is the same for cases (d) and (e), due to the fact that the bandwidth is the same for these two cases if $\Gamma=0$. $l(E)$ does not then reflect the difference between the number of closest nearest neighbors of the two different lattices.

Case (f). For a Bethe lattice,

$$\kappa=\ln(Z_n-1)^{1/2}+\kappa_1\ . \tag{8}$$

Here Z_n is the number of nearest neighbors. κ_1 has the form (6) with $E_S=2(Z_n-1)^{1/2}V$ and

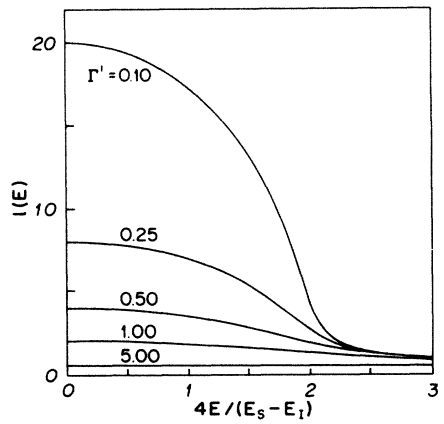

FIG. 1. The attenuation length $l \equiv \kappa^{-1}$ as a function of energy in units of $(E_S - E_I)/4$, for the different lattices which were considered except for the square lattice in the (1,1) direction (see Fig. 2). Γ is the disorder parameter measured in the same units as the energy. See discussion in the text for the definition of E_S and E_I in the cases (a), (c), (d), (e), and (f). Lengths are in units of nearest-neighbor distance.

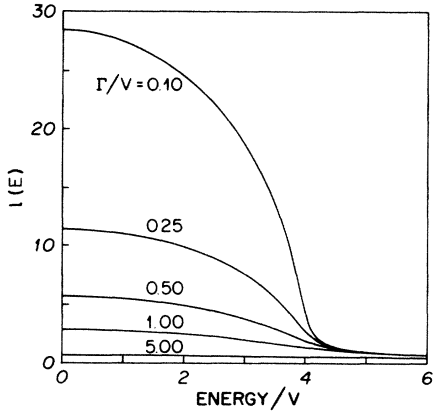

FIG. 2. The attenuation length $l = \kappa^{-1}$ as a function of energy for a square lattice in the (1,1) direction. Energy is in units of the hopping parameter V and lengths are expressed in units of the nearest-neighbor distance. Γ is the disorder parameter.

$E_I = -2(Z_n - 1)^{1/2}V$. The term in $\ln(Z_n - 1)^{1/2}$ is present even if $\Gamma = 0$ and reflects the fact that the number of sites separated from a given site grows with distance R as $\exp[(Z_n - 1)R]$.

DISCUSSION

Two factors contribute to the decay of $\langle G_{0,\mathbf{R}}(E)\rangle_{\text{av}}$ as a function of R: the decrease of the modulus of $G_{0,\mathbf{R}}(E)$ for each member of the ensemble, and the result of interference in the average due to random phases of $G_{0,\mathbf{R}}$ for different members of the ensemble.

Let us assume that we are in a range of energies and disorder for which the states are extended. For each system of the ensemble, $G_{0,\mathbf{R}}$ as a function of $\mathbf{R}$ will be of the order of $R^{(1-d)/2}$, which is not sufficient to give an exponential decrease (except for a Bethe lattice). However, the disorder causes random phases in $G_{0,\mathbf{R}}$ among different systems of the ensemble, which do give rise to an exponential decrease in $\langle G_{0,\mathbf{R}}\rangle_{\text{av}}$. Due to this reason, $l(E)$ can be associated with a phase-coherence length.[10] This identification is less precise as we get close to a mobility edge, where fluctuations in $|G_{0,\mathbf{R}}(E)|$ may contribute, along with random phases, to the decrease of the average. Following Abrikosov *et al.*,[11] one can interpret $l = \kappa^{-1}$ as a mean free path for $|\mathbf{k}\rangle$ state. For energies close to the band center and $\Gamma/(E_S - E_I) \ll 1$, for any of the considered three-dimensional lattices, one has $l \simeq (E_S - E_I)/(2\Gamma)$.

On the other hand, the exponential decay of $|G_{0,\mathbf{R}}|$ for each system is uniquely associated with localization of states.[7,8] One expects that in the region of strongly localized states, the exponential decay of $\langle G_{0,\mathbf{R}}\rangle_{\text{av}}$ is principally due to localization so that $\kappa(E) \simeq \gamma(E)$. Close to a band edge, for an arbitrary lattice, one has

$$\gamma(E) \simeq \kappa(E) \simeq \left[\frac{2m^*}{\hbar}\left[\frac{[(E-E_S)^2+\Gamma^2]^{1/2}+(E-E_S)}{2}\right]\right]^{1/2}, \tag{9}$$

where m^* is the effective mass[12] for the band edge. The above discussion is schematically illustrated in Fig. 3. There, we show the regions where amplitude and phase fluctuations are present.

In the cases we have studied with $d > 1$, $\kappa(E)$ always depends on E and d throughout the entire energy range. Also, $\kappa(E=0)$ decreases when the dimensionality of the system is increased. From the above discussion it is seen that $\kappa(E)$ is an upper bound for $\gamma(E)$ so that $\kappa(E) > 0$ does not imply localization of states.

However, for a linear chain $(d=1)$, one has $\kappa(E) = \gamma(E)$,[3-5] which gives only one characteristic length

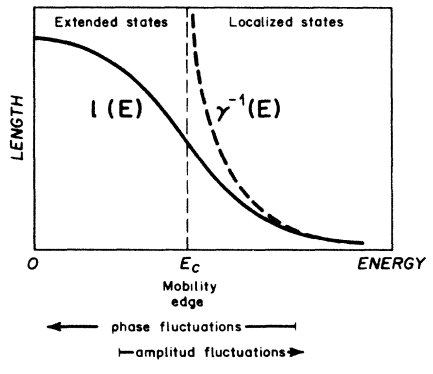

FIG. 3. Schematic illustration of the length $l = \kappa^{-1}$ showing its behavior as a function of energy in a hypothetical case where there is a mobility edge E_c. We indicate the regions where the fluctuations in the phases or amplitudes of $G_{0,\mathbf{R}}(E)$ would be important. The localization length $\gamma^{-1}(E)$ is also shown in the figure.

in this case. Also, in the case of one-dimensional binary alloys, recent results[13] for the length associated with the exponential decrease of $\langle G_{0,\mathbf{R}}(E)\rangle_{\mathrm{av}}$ agree very well with the numerical calculation of the localization length. Therefore, this might always be true in one dimension (1D) and come from the same reasons which permit one to write $\gamma(E)$ as a function of the total density of states in one dimension.[3] In the case of the Lorentzian distribution there is another reason which makes plausible the statement that the exponential decrease of $\langle G_{0,\mathbf{R}}(E)\rangle_{\mathrm{av}}$ in 1D is essentially due to localization. Stone *et al.*[14] has shown that for a one-dimensional system with a rectangular distribution of site energies, the phase coherence of $G_{0,\mathbf{R}}(E)$ is maintained up to an arbitrary distance in the case of strong disorder. Keeping in mind that the fluctuations due to the Lorentzian disorder will effectively break the linear chain into nearly isolated segments, this disorder can always be considered strong.[15] Therefore it seems reasonable that random phases should not play a very central role here.

The point which remains to be discussed is the observation, already made in the second section, that $\kappa(E)$ has the same expression as that deduced by JK to calculate $\gamma(E)$. If these quantities were equal, it would mean that all the scattering processes that contribute to the phase incoherence of $G_{0,\mathbf{R}}$ also contribute with the same efficiency to the localization. Even when this is the case for one-dimensional systems, it is strange that the localization length does not depend on the dimensionality for energies close to the band center. This leads us to suspect that the quantity calculated by JK was not in fact the localization length.

The starting assumption in the work of JK is that the minimum Lyapunov characteristic exponent can be evaluated as

$$\lim_{R\to\infty}\left[-\frac{1}{R}\lim_{\delta\to 0}\langle \ln|\, G_{0,\mathbf{R}}(E+i\delta)\,|\,\rangle_{\mathrm{av}}\right], \tag{10}$$

which differs from (2) in the fact that the ensemble average is done *before* taking the limit $\delta\to 0$. The crucial point is that different orders in that limit may not produce the same result. So the mistake at this point is the same as that made by Lloyd[1] when he considered that

$$\lim_{\delta\to 0}\langle \mathrm{Im}G_{\mathbf{R},\mathbf{R}}(E+i\delta)\rangle_{\mathrm{av}}=\mathrm{Im}G^{0}_{\mathbf{R},\mathbf{R}}(E+i\Gamma)<0 \tag{11}$$

implied quantum diffusion and therefore provided evidence for the existence of extended states. The later work of Ishii[4] proved that in order to study localization, one must evaluate

$$\langle \lim_{\delta\to 0}\mathrm{Im}G_{\mathbf{R},\mathbf{R}}(E+i\delta)\rangle_{\mathrm{av}}, \tag{12}$$

which is zero if and only if the spectra has no absolutely continuous part. In this case quantum diffusion, if it exists, is slow.

In fact, following Ref. 5 it is not difficult to show that for a one-dimensional system $G_{\mathbf{R},\mathbf{R}}$ is a real number and has a Lorentzian distribution with a mean given by

$$\begin{aligned}\langle G_{\mathbf{R},\mathbf{R}}(E)\rangle_{\mathrm{av}}&=\langle \lim_{\delta\to 0}G_{\mathbf{R},\mathbf{R}}(E+i\delta)\rangle_{\mathrm{av}}\\&=\mathrm{Re}\lim_{\delta\to 0}\langle G_{\mathbf{R},\mathbf{R}}(E+i\delta)\rangle_{\mathrm{av}}\\&=\mathrm{Re}G^{0}_{\mathbf{R},\mathbf{R}}(E+i\Gamma),\end{aligned} \tag{13}$$

and a width given by $\mathrm{Im}G^{0}_{\mathbf{R},\mathbf{R}}(E+i\Gamma)$. The second equality holds only for the infinite 1D system. However, it illustrates the more general situation in which the analytical continuation of an average evaluated on the complex plane, which is itself a complex quantity, does not coincide with the average evaluated on the real axis. The first procedure is appropriate in order to study the rough features of the distribution of states, but cannot distinguish among absolutely continuous and singular spectra. Thus, in order to study localization one must analyze either the $\delta\to 0$ limit of the Green's function of a particular system, or the ensemble average of the Green's functions already evaluated on the real axis.

The nonuniformity in the average and the limit $\delta\to 0$ is responsible for the misleading results of JK. This can be appreciated, for example, in their formula A(2.8), which states

$$\mathrm{Tr}\langle(z\hat{1}-\hat{\mathscr{H}})^{-1}\rangle_{\mathrm{av}}=\mathrm{Tr}\langle G^{0}(z+i\Gamma)\rangle\ .$$

According to the previous discussion, the last equality is not valid if the value $\delta=0$ is taken before the average. From this we conclude that the initial assumption of JK in using formula (10) is responsible for the fact that κ rather than γ was found.

This conclusion is also supported by their own numerical simulations. They found that the value of γ taken from the numerical simulation is always smaller than their theoretical value. Moreover, the discrepancy between both values became stronger as Γ or E diminished; this is in agreement with our interpretation.

Our conclusion that previous proof of localization in the Lloyd model is not valid opens again the question about what really occurs with the eigenstates in this model. Even when we were not able to prove the existence of extended states for $d>2$, there is a physical argument that suggests that even when the Lorentzian distribution does not have finite moments, the system could have extended states. This follows from the fact that we could exclude from the calculation all the lattice sites with diagonal term of magnitude greater than a certain ε_M. If we choose a large enough ε_M, the concentration p of the remaining sites will be above the percolation threshold and their energy distribution will have a finite moment. As Γ decreases, these moments decrease and p increases. Then the quantum interference effect will be less significant[16] allowing for the existence of extended states if $d>2$.

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