Universal behavior near the band edges for disordered systems: Numerical and coherent-potential-approximation studies

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The integrated densities of states (DOS) of one-, two-, and three-dimensional tight-binding models with diagonal and off-diagonal disorder are calculated numerically. Our results for the diagonal-disorder case confirm the expected universal behavior of the DOS, particularly near the band edges. The simple exponential behavior of the DOS is clearly displayed in the three-dimensional results. The off-diagonal-disorder case follows a universal behavior too, which agrees reasonably well with the coherent-potential-approximation (CPA) results. Our results are compared with the various phenomenological theories, with the CPA conclusions, and with previous numerical results.

I. INTRODUCTION

From the optical-absorption coefficient measurements on crystalline and amorphous semiconductors and crystalline insulators, it has been deduced that the absorption coefficient α often exhibits (over a limited range of energies) an exponential behavior of the form

$$\ln\alpha \sim (E - E_f)/E_0 , \tag{1.1}$$

known as the Urbach tail.[1] E_f is the so-called Urbach focus and E_0 determines the slope of the curve of $\ln\alpha$ versus $E = \hbar\omega$; ω is the photon frequency. The quantity E_0 is of the order of 50 meV or less, the higher values appearing in amorphous materials.[2] Many theories have been proposed[3-10] to explain the rather general exponential behavior shown in Eq. (1.1). Most of them attribute the frequency dependence of α to an exponential tail in the density of states (DOS) in the top of the valence band and/or the bottom of the conduction band. Various physical mechanisms have been assumed and different formalisms have been employed in order to obtain the exponential tail in the DOS. This proliferation of formalisms and detailed physical mechanisms tend to obscure the common feature of a fluctuating potential being the source of the exponential tails in the DOS.

Recently, Monroe and Kastner[11] have demonstrated through transient photocurrent measurements in glassy As_2Se_3 that the DOS appears to exhibit exponential tails over a rather extended energy range from 0.3 to 0.86 eV above the valence band.

The rather general character of the exponential tails in the DOS suggests a quasiuniversal mechanism that bypasses the complexity of real materials. In our quest[12,13] for uncovering such possible underlying quasiuniversality, we have reached the conclusions that the behavior of the DOS (and other quantities of physical interest) near the band edge depends on the following.

(i) The DOS $\rho_0(E)$ corresponding to the periodic Hamiltonian $H_0 \equiv \langle H \rangle$.

(ii) The standard deviation w^2 of the independent local contributions ε_n to the fluctuating part of the Hamiltonian $H - \langle H \rangle$.

(iii) The tail of the probability distribution $p(\varepsilon_n)$.

The last plays an important role in determining the tails in the DOS. If many independent physical mechanisms are responsible for the fluctuation of each ε_n, then one expects that the distribution $p(\varepsilon_n)$ will be Gaussian, i.e.,

$$p(\varepsilon_n) = \frac{1}{\sqrt{2\pi}w} \exp\left[\frac{-\varepsilon_n^2}{2w^2}\right] . \tag{1.2}$$

We have shown[13] by second-order perturbation theory or the coherent-potential approximation (CPA) that the fluctuating local potentials will produce an almost rigid shift of the "unperturbed" DOS $\rho_0(E)$ by an amount which is proportional to w^2. Once the energies are measured relative to the CPA band edge, all the physical quantities of interest, including the DOS, are universal, provided that the length and energy are scaled relative to disorder-dependent units of energy and length.[12,13] This universality holds for the Halperin-Lax (HL) regime[4] and the regime close to the CPA band edge. Note that the energy width of the HL regime in three dimensions is very narrow, typically less than 50 meV. The universality breaks down on the extended regime as the energy approaches the nearest Van Hove singularity inside the band and on the localized regime when the localization takes place by narrow deep potential fluctuations. This regime is described well by elementary quantum-mechanical considerations or by the CPA, and when coupled with Gaussian disorder, it exhibits an exponential behavior which is seen experimentally in the absorption coefficient. The physical origin of the exponential behav-

ior is the simple fact that the binding energy $|E|$ in a potential well is a linear function of ε^2, i.e., $|E| = A\varepsilon^2 + B$, where ε is the depth of the potential well. This simple relation is valid in the regime where the decay length of the bound state is comparable to the linear extent of the potential well.[14] Since the depth of the potential well is assumed to have a Gaussian probability distribution $p(\varepsilon) \sim \exp(-\varepsilon^2/2w^2)$, it follows immediately that the DOS will exhibit an exponential behavior

$$\rho(E) \sim \exp\left[-\frac{|E|}{2Aw^2}\right] . \tag{1.3}$$

The energy width of this exponential behavior is much wider than the HL regime, in accordance with experiment.[2,11] The exponential behavior could span more than 5 orders of magnitude. Finally much deeper into the tail we obtain, as we should, a gradual change of the behavior of the DOS which approaches the same functional form as the probability distribution for the disorder. This limiting behavior cannot easily be seen because it is very deep into the tail. Similar results[10] have been obtained by a sophisticated and powerful formulation which is based upon the replica field theory representation of the averaged one-electron Green's function.[9,10] An asymptotically exact DOS may be obtained by saddle-point evaluation of the relevant functional integral. The nontrivial saddle points[15] (instantons) reveal the nature of both the most probable potential fluctuation and the corresponding bound-state wave function at any fixed energy $-|E|$.

While the ideas vary, the implicit basic position is that the exponential tail of $\rho(E)$ should be explainable solely on the basis of random potential fluctuations. Therefore, it is very important to obtain numerically the true DOS behavior in one-, two-, and three-dimensional (1D, 2D, and 3D) disordered systems[16,17] to check the universality ideas, the widths of the HL and the simple exponential, as well as the predictions of the CPA. In this work, we have used the Sturm sequence method[18] to calculate the integrated DOS in 1D, 2D, and 3D tight-binding Hamiltonians with Gaussian distribution of site energies. We have also studied the role of the off-diagonal disorder on the behavior of the DOS in the tail region, and checked if the universality obtained for the diagonal disorder is still retained here.

In Sec. II, we briefly described the formalism and the method of calculation. In Sec. III, we present and discuss the results of this calculation and in the final section, we state the conclusions of this work.

II. THE THEORETICAL FRAMEWORK

We consider the tight-binding model with either diagonal or off-diagonal disorder,

$$H = \sum_n \varepsilon_n |n\rangle\langle n| + \sum_{[n,m]} V_{nm} |n\rangle\langle m| , \tag{2.1}$$

where the sites n form a regular lattice (square in two dimensions and simple cubic in three dimensions) of lattice constant a. $[n,m]$ denotes the nearest-neighbor pair and ε_n is the random site energy (diagonal disorder) which is Gaussian distributed with mean zero and variance w^2 and $V_{nm} = V$. The use of Gaussian distribution for ε_n is based on the reasonable assumption, supported by experiment,[2] that fluctuations of ε_n arise from many independent physical mechanisms. For the pure off-diagonal-disorder case, the matrix elements V_{nm} are random variables and ε_n constant. The logarithm of the V_{nm} is given by a rectangular probability of width W_0. W_0 is a good measure of the strength of the off-diagonal disorder.[19]

For the case of the diagonal disorder, the CPA calculates the average (i.e., the arithmetic mean) Green's function corresponding to H from an effective periodic Hamiltonian resulting from Eq. (2.1) by replacing each ε_n by a common self-energy Σ, which is determined by the following equation,[20]

$$\Sigma(E) = \int d\varepsilon_n p(\varepsilon_n) \frac{\varepsilon_n}{1-(\varepsilon_n - \Sigma)G_0(E-\Sigma)} , \tag{2.2}$$

where $G_0(E)$ is the diagonal element of the unperturbed Green's function in which all the ε_n's are the same. For relatively weak disorder[12] $wG_0 \ll 1$, one can expand Eq. (2.2) to obtain

$$\Sigma = w^2 G_0(E-\Sigma) - (2w^4 - \mu_4) G_0^3(E-\Sigma) , \tag{2.3}$$

where $\mu_4 = \int \varepsilon_n^4 p(\varepsilon_n) d\varepsilon_n$ is the fourth moment of the distribution. For rectangular distribution $2w^4 - \mu_4 = w^4/5$ and for the Gaussian case, $2w^4 - \mu_4 = -w^4$. Equation (2.3), together with the expression of $G_0(E)$ near the band edge was used successfully to obtain the quasiuniversal behavior of the DOS and the other quantities of interest near the band edges,[12] It is known that a reasonable approximation to the DOS in the whole energy range can be obtained by the CPA when supplemented by the appropriate HL behavior outside the pure band edge.[12,16]

The off-diagonal-disorder case can be also treated by the CPA. Most of the efforts[20] obtained a solution to the problem for the case of the binary distribution by introducing a 2×2 matrix version of the simple CPA equation. We have used the homomorphic cluster CPA developed by Yonezawa and Odagaki[21] to obtain the corresponding equation to Eq. (2.3) for the off-diagonal disorder. It has been shown[21] that this cluster CPA produces analytical Green's functions but is only right for the case of pure off-diagonal disorder. Using the CPA condition for a two-site cluster, we obtained, after some algebra that (the details are given in the Appendix)

$$\Sigma' = w_e^2 G_0(E' - \Sigma') , \tag{2.4}$$

where

$$E' = (1 + w_0^2/2d)E , \tag{2.5a}$$

$$\Sigma' = (1 + \alpha E^2/2d)\Sigma , \tag{2.5b}$$

$$w_e^2 = (1/\alpha + E^2/2d)w_0^2 , \tag{2.5c}$$

and d is the space dimensionality, w_0 is defined in Eq. (A9), and $\alpha = 1/n$ where n is the number of nearest neighbors. Notice that Eq. (2.4) is exactly the CPA equation (2.3) to order w^2. Hence, any results we have obtained

for the diagonal-disorder case[12] can be equally applied to the off-diagonal disorder with the rescaling equation (2.5). For the 1D tight-binding model with off-diagonal disorder, Mielke and Wegner[22] have calculated in the limit of weak disorder at the band edge the DOS and the localization length. After rescaling their results with Eq. (2.5c), they obtained the universal behavior given for the diagonal-disorder case by Derrida and Gardner.[23] This behavior has been confirmed numerically both for the diagonal[13,17] and off-diagonal case.[24]

We have used the Sturm sequence method to calculate the integrated DOS.[25] The method consists of an application of the Gaussian elimination trick on the consecutive columns or rows of the matrix $(E\underline{1}-\underline{H})$ where E is an energy and $\underline{1}$ a unit matrix of the same size as H. The Gaussian elimination of the elements of the matrix is applied until the matrix is reduced to a triangular form. The integrated DOS is then calculated by counting the fractional number of positive elements in the diagonal of the reduced triangular matrix.[26] For details of how to perform these calculations, see Refs. 25 and 26. The advantage of using this method is both economy in storage and speed. The computing time rises as $M^{3(d-1)}\times N$ which allows us to consider very long strips of considerable width. It also does not require matrix inversion and working with real numbers speeds up the calculation. In our calculations, we have used systems as large as 1×10^7 for the 1D case, 50×4000 for the 2D case, and $10\times10\times400$ and $20\times20\times100$ for the 3D case. The accuracy of our calculations is very good, varying from 1% close to the band edge to 10% in the deep tail.

III. RESULTS AND DISCUSSION

We show in Fig. 1(a) the integrated DOS [IDOS or $I(E)$] for a 2D tight-binding model with diagonal disorder of Gaussian type with standard deviation w^2 for four values of w. Notice that the IDOS clearly displays an exponential behavior of the form $\exp(-E/E_0)$, where E_0 depends approximately linearly on the second power of disorder. Following Eq. (1.3) we have that $E_0=2Aw^2$. The value of A predicted analytically from the HL theory[4,15] is $A=1/(8\pi)0.9311=0.0427$ and, from the path-integral formalism[10] $A=1/8\pi=0.0398$. We find the following values for A, 0.0427, 0.0625, 0.0694, 0.0571, and 0.0532, for values of disorder $w=3$, 2, 1, 0.5, and 0.25, respectively. The values of A slightly depend on disorder, but within 30% agree with the analytical results. We want to mention that the CPA will also give an exponential behavior[12] for the IDOS. For the 2D square lattice close to the band edge, we have that $1/G_0^2(E)=4-11.66E$, where E is measured from the unperturbed band edge of 4 in units of V and $G_0(E)$ is the Green's function for the periodic 2D tight-binding lattice. Following Eq. (2.7) of Ref. 12, we obtain $\rho(E)\sim\exp(-E/E_0)$ and $E_0=2Aw^2$, where $A=0.0857$ which is roughly twice as large as the HL value and the path-integral formalism predictions. In Fig. 1(b), we replot the data that are presented in Fig. 1(a), but after a scaling of the DOS and E that was suggested in Ref. 12 we have for the 2D system that

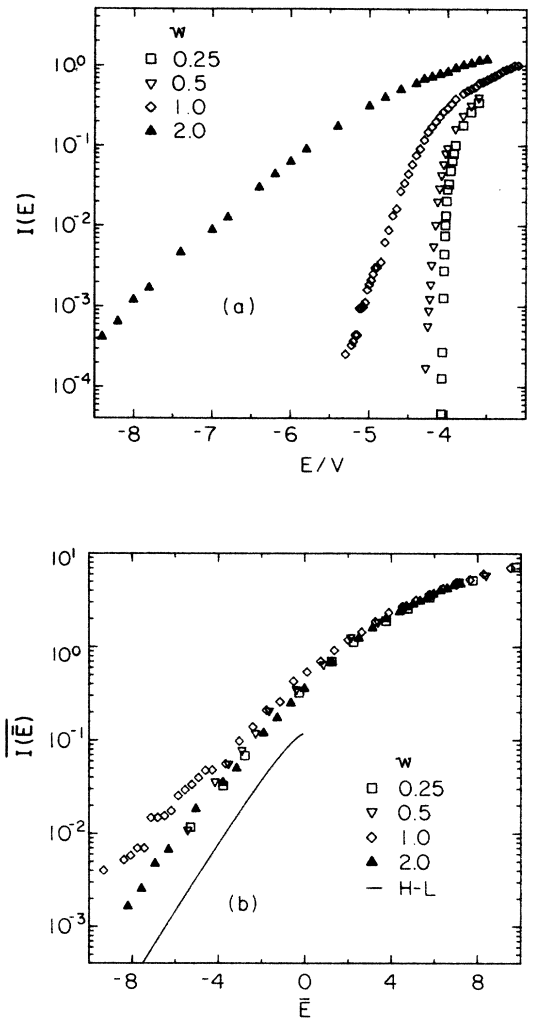

FIG. 1. (a) Plot of the tail-integrated density of states $I(E)$ as a function of energy E for the 2D tight-binding model with Gaussian diagonal disorder of strength w. (b) Plot of the 2D scaled tail-integrated density of states $\overline{I(\bar{E})}$ as a function of the scaled energy. $\overline{I(\bar{E})}=I(E)\times L_{02}^2$, $\bar{E}=(E-E_{\rm CPA})/\varepsilon_{02}$, where $\varepsilon_{02}=w^2/4\pi V$, $L_{02}=(4\pi V/w)a$. The solid line is the universal curve of Halperin-Lax theory (Refs. 4 and 12). The maximum size of systems is 50×4000.

$$\bar{\rho}(\bar{E})=0.120\bar{E}^{\,0.5689}\exp(-0.9311\bar{E})\,, \tag{3.1}$$

where $\bar{\rho}=\rho4\pi Va^2$ and $\bar{E}=(E-E_{\rm CPA})4\pi V/w^2$ and $E_{\rm CPA}$ is the CPA band edge determined as the truncated CPA equation (2.3). For the 2D case, we have that[16]

$$E_{\rm CPA}=-4V-\frac{w^2}{2\pi V}\left[\ln\left[\frac{w}{8\sqrt{2\pi}V}\right]-\frac{1}{2}\right]. \tag{3.2}$$

Notice that all the different disorder cases fall into one universal curve, which is a little higher than the integration of Eq. (3.1). In the 2D case, the HL theory as well as the CPA predict that the DOS will behave exponentially and therefore the universality[12] is easily observed. Only for strong disorder $w=3.0$, there is a deviation from the

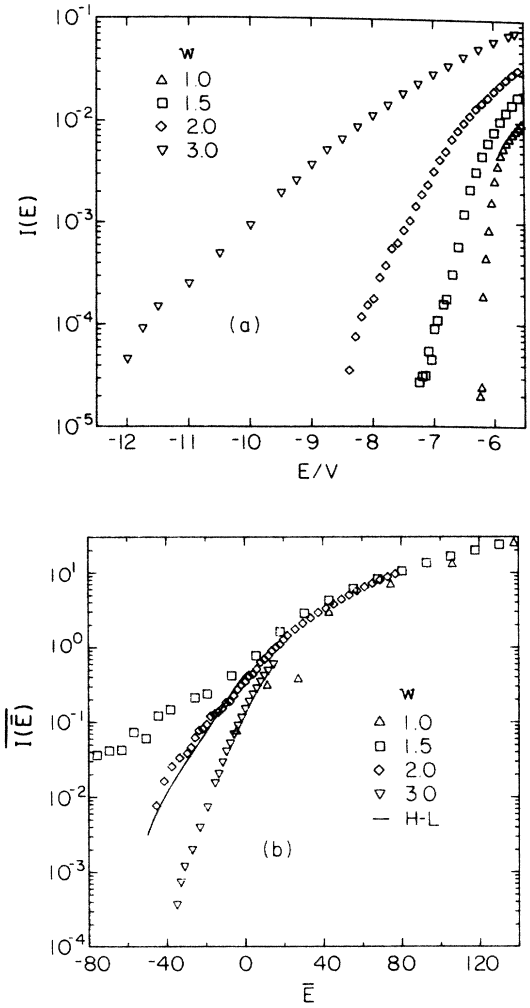

FIG. 2. (a) Plot of the tail-integrated density of states $I(E)$ as a function of energy E for the 3D tight-binding model with Gaussian diagonal disorder of strength w. (b) Plot of the 3D scaled tail-integrated density of states $\overline{I(\bar{E})}$ as a function of the scaled energy $\bar{E}$. $\overline{I(\bar{E})}=I(E)\times L_{03}^3$, $\bar{E}=(E-E_{\rm CPA})/\varepsilon_{03}$, where $\varepsilon_{03}=w^4/(8\pi)^2V^3$, $L_{03}=(8\pi V^2/w^2)a$. The solid line is the universal curve of Halperin-Lax theory (Refs. 4 and 12). The maximum size of systems is $10\times10\times3000$.

universality.

In Fig. 2(a), we present four sets of 3D integrated DOS's calculated on a simple-cubic lattice with $w=1$, 1.5, 2, and 3. Notice that our numerical results provide for the first time clear evidence in support of an exponential behavior $\exp(-E/E_0)$ in agreement with the CPA predictions[12] and the path-integral formalism.[10] The value of A in the formula $E_0=2Aw^2$ is given by $A=0.0417$, 0.0476, 0.0403, and 0.0333 for $w=3.0$, 2.0, 1.5, and 1.0, respectively. There is again a disorder dependence of A, but they qualitatively agree with the predictions of the CPA (Ref. 12) that give a value of $A=0.06$ predicted analytically on the basis of an asymptotic equation.[12] We have also numerically calculated[12] A within the CPA for the 3D tight-binding model with Gaussian disorder for a cubic lattice as well as for the Hubbard model.[3] The values of A range from 0.06 for small w to $A=0.04$ for large disorder.[12] It is clear from our numerical results for three dimensions that the HL region is much narrower than the exponential regime, in accordance with experiment[11] and the path-integral formalism.[10] It was clearly shown in Ref. 10 that the range of the exponential behavior of the DOS, which gives a value of $A=\frac{1}{2}(14.4)\pi=0.011$ is much wider than the HL regime.[14] Numerical results for the 3D diagonal disorder were also presented by Zhang and Sheng.[17] They have used the recursion method[17] to calculate the DOS, which probably is not so accurate for the small-disorder cases and deep into the tail. Around the CPA band edge, which is the HL region, we have agreement between the two methods, but deep into the tails, which supposedly gives the exponential behavior, there is disagreement. This is reflected in the fact that values of A that they are getting are too small for all the disorders w less than 1.5 (i.e., $A\leq0.01$). Only for $w=1.8$, $A=0.03$. It is the integrated DOS that gives much more accurate results and, therefore, we are able to check the exponential behavior of the DOS. We replot in Fig. 2(b) the data from Fig. 2(a) with the scaling of DOS and E suggested in Ref. 12. One sees that the universality is obeyed only for small disorder and only close to the CPA band edge. To make this point clear and also to show that the CPA correctly describes the behavior of the DOS in most of the regions of interest, we replot the numerical data and the CPA results of Ref. 17 before they were scaled. This is shown in Fig. 3. Notice that for $w=1.2$, 1.5, and 1.8, the numerical results and the CPA results agree reasonably well. For small disorder, $w=0.9$, which is the worst case for the CPA, we find, in fact, that the CPA misses some of the states for $E\geq6.20$. There the CPA has to be supplemented by the HL behavior of DOS.[4,12] Notice from Fig. 3 that the results of Ref. 17, if they are plotted

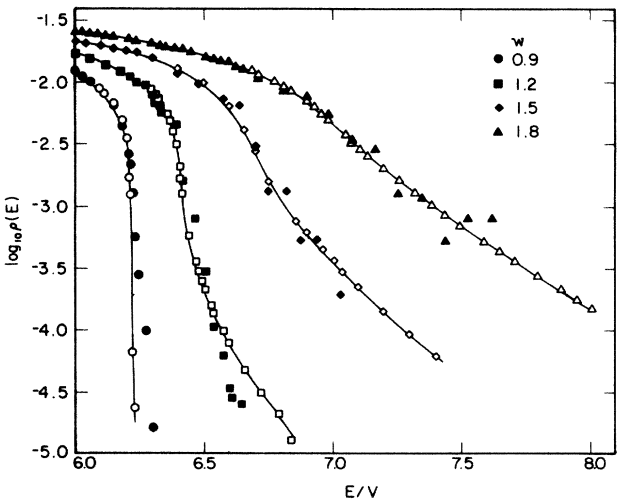

FIG. 3. Plot of the density of states ρ or the 3D tight-binding model with Gaussian diagonal disorder of strength w. Empty symbols are CPA results and solid symbols are numerical results of the recursion method (data are taken from Fig. 3, Ref. 17).

without any scaling, do not exaggerate the difference between the CPA calculation and the numerical results. The same is also true for the 2D diagonal results of Ref. 17.

For completeness we also plot in Fig. 4(a) the results of the IDOS versus E for the 1D diagonal-disordered case with $w=0.02$, 0.2, 0.5, and 1.0. Notice in Fig. 4(b) that all the diagonal-disorder results replotted with the appropriate scaling of energy and DOS follow the universal behavior predicted for one dimension.[4,13,23] The universality breaks down deep into the tail ($E<-4.25$) for large enough disorder.

We have also calculated the IDOS for 2D and 3D tight-binding disordered systems with only off-diagonal disorder. Up to now, most of the numerical work as well as the analytical work has been done for the diagonal case. The off-diagonal-disorder case is very useful in deciding whether or not all of the universal features near the band edges seen in the diagonal case will be also present in this case too. It is also very interesting to check if the DOS has a simple exponential behavior in the presence of the off-diagonal disorder. We have taken that the logarithm of the nearest-neighbor off-diagonal matrix elements are randomly distributed with a rectangular distribution of width W_0 The standard deviation w_0 for this probability distribution is proportional to W_0. We have used $w_0^2=(\langle V^2\rangle-\langle V\rangle^2)/\langle V\rangle^2$. In Fig. 5(a), we plot the IDOS versus E for five values of the off-diagonal-disorder $W_0=0.10$, 0.25, 0.50, 1.0, and 2.0. Notice that in this case the IDOS does not give a clear exponential behavior as it did for the diagonal case. However, if we assume $E_0=2Aw_e^2$, the IDOS is proportional to $\exp(-E/E_0)$ and by doing the rescaling [Eq.

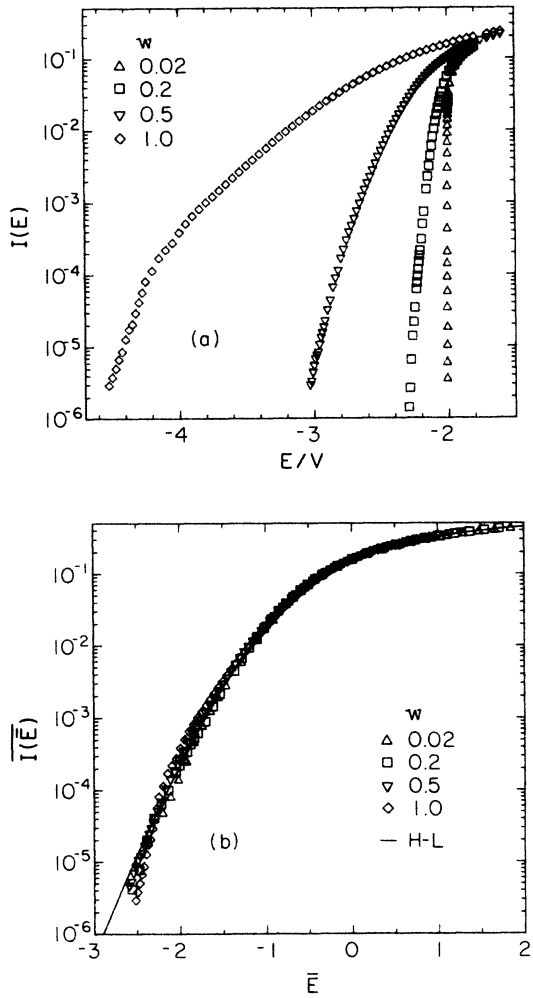

FIG. 4. (a) Plot of the tail-integrated density of states $I(E)$ as a function of energy E for the 1D tight-binding model with Gaussian diagonal disorder of strength w. (b) Plot of the 1D scaled tail-integrated density of states $\overline{I(\bar{E})}$ as a function of the scaled energy $\bar{E}$ for diagonal disorder, $\overline{I(\bar{E})}=I(E)\times L_{01}$ $\bar{E}=(E-2V)/\varepsilon_{01}$, where $\varepsilon_{01}=w^{4/3}/V^{1/3}$, $L_{01}=(V^{2/3}/w^{2/3})a$. The solid line is the universal curve of Halperin-Lax theory (Refs. 4 and 12). The maximum size of systems is 5×10^6.

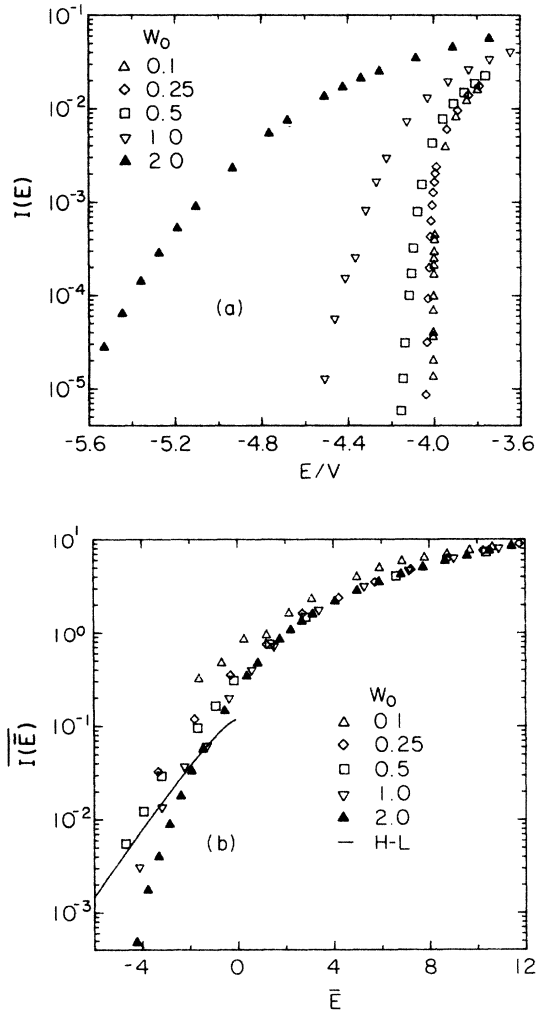

FIG. 5. (a) Plot of the tail-integrated density of states $I(E)$ as a function of energy E for 2D pure off-diagonal disorder of strength W_0. (b) Plot of the scaled tail-integrated density of states $I(\bar{E})$ as a function of scaled energy $\bar{E}$ for 2D pure off-diagonal disorder. $\overline{I(E)}=I(E)\times L_{02}'^2$, $\bar{E}=(E'-E_{\rm CPA})/\varepsilon_{02}'$, where $\varepsilon_{02}'=w_e^2/4\pi V$, $L_{02}'=(4\pi V/w_e)a$ and E', w_e are defined in Eqs. (2.5a)–(2.5c). The solid line is the universal curve of Halperin-Lax theory (Refs. 4 and 12). The maximum size of systems is 50×6000.

(2.5c)], the results for the off-diagonal case must agree with those of the diagonal case. For the 2D off-diagonal case, we have the effective standard deviation $w_e^2=8w_0^2$. We have from our numerical results that $A=0.022$, 0.042, 0.047, 0.065, and 0.094 for $W_0=2.0$, 1.0, 0.5, 0.25, and 0.10. Notice that the values of A agree reasonably well with that obtained for the diagonal case discussed above. In Fig. 5(b), we replot our numerical data, shown in Fig. 5(a) by doing the appropriate scaling of DOS and energy suggested in Ref. 12, as well as the scaling [Eq. (2.5c)] for the effective standard deviation w_e, and [Eq. (2.5a)] for the energy. Notice that all different off-diagonal-disorder cases fall into a universal curve, which again is a little higher than the integration of Eq. (3.1). From these analysis, we conclude that the off-diagonal-disorder case is very similar to the diagonal case if we do

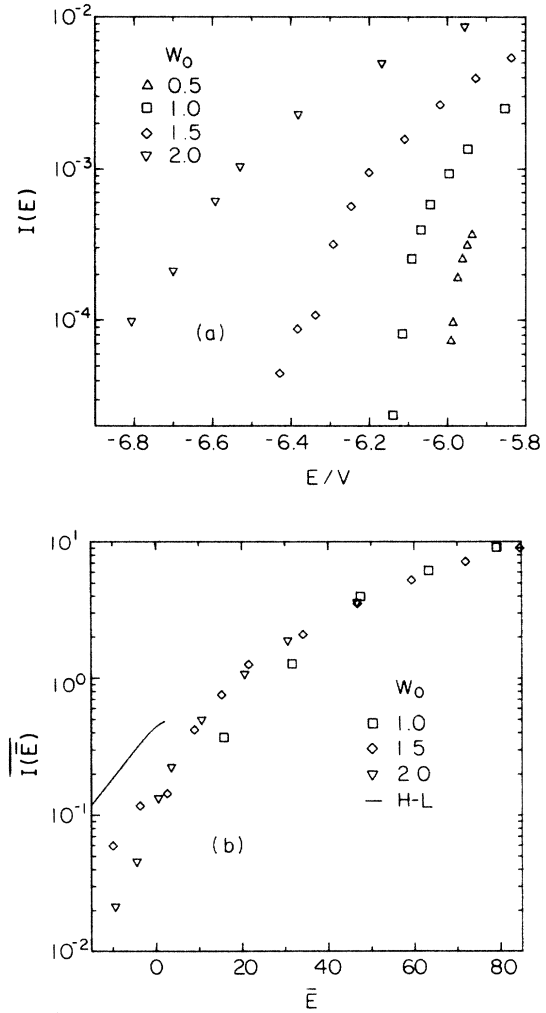

FIG. 6. (a) Plot of the tail-integrated density of states $I(E)$ as a function of energy E for 3D pure off-diagonal disorder of strength W_0. (b) Plot of the scaled tail-integrated density of states $\overline{I(\bar{E})}$ as a function of the scaled energy $\bar{E}$ for 3D pure off-diagonal disorder. $\overline{I(\bar{E})}=I(E)\times L_{03}'^3$, $\bar{E}=(E'-E_{\rm CPA})/\varepsilon_{03}'$, where $\varepsilon_{03}'=w_e^4/(8\pi)^2V^2$, $L_{03}'=(8\pi V^2/w_e^2)a$, and E', w_e are defined in Eqs. (2.5a)–(2.5c). The solid line is the universal curve of Halperin-Lax theory (Refs. 4 and 12). The maximum size of systems is $20\times20\times150$.

the scaling shown in Eqs. (2.5a)–(2.5c) for the energy E, the self-energy Σ, and the standard deviation w_e. Of course, these findings are only correct to the w^2 order within the CPA and expected to break down when the off-diagonal disorder w_0 becomes large.

In Fig. 6(a), we plot the results for the 3D tight-binding model with only off-diagonal disorder for values of $W_0=2.0$, 1.5, 1.0, and 0.5. As in the 2D off-diagonal case the 3D IDOS versus E does not exactly behave as a simple exponential. It looks like the IDOS versus E drops faster than the exponential. However, if we assume that the IDOS is proportional to $\exp(-E/E_0)$ with $E_0=2Aw_e^2$ and by doing the rescaling [Eq. (2.5c)], the results for the off-diagonal case must agree with those of the diagonal case. For the 3D off-diagonal-disorder case, we have the effective standard deviation $w_e^2=12w_0^2$. We have from our numerical results $A=0.016$, 0.017, 0.01, and 0.033 for $W_0=2.0$, 1.5, 1.0, and 0.5. The values of A agree reasonably well with those obtained for the diagonal case. Of course in this case too, the value of A depends on a disorder which suggests the assumption that IDOS is proportional to $\exp(-E/E_0)$ is not completely correct.

In Fig. 6(b), we replot the results shown in Fig. 6(a) by doing the appropriate scaling of DOS and energy suggested in Refs. 12 and 17. To connect the off-diagonal results with the diagonal we have to also scale the energy by Eq. (2.5a) and the standard deviation by Eq. (2.5c). Notice that all the different off-diagonal-disorder results fall into a universal curve. We might say that the 3D off-diagonal results follow the universal behavior better than the results for the 3D diagonal case. The exponential behavior of the IDOS for the 3D off-diagonal case is not well established from our data.

For completeness and a check of our numerical method, we also calculated the IDOS for the 1D off-diagonal-disordered system with $W_0=0.02$, 0.2, 0.5, 1.0, and 2.0. These results are shown in Fig. 7(a). Notice that, as expected for the 1D case, the IDOS versus E does not follow a simple exponential. However, by the appropriate scaling of energy and DOS, as well as the scaling in Eq. (2.5), we obtain that all the data follow a universal curve. This is clearly shown in Fig. 7(b), where the solid line is the HL universal prediction for the 1D case and almost all the data for small disorder W_0 follow this line. Of course, if disorder is large enough, we start having deviations from the universality as one gets into the far tail of the IDOS. Similar results were obtained in Refs. 22 and 24 for very small disorders.

IV. CONCLUSIONS

We have performed detailed numerical results for the IDOS for 1D, 2D, and 3D tight-binding models with only diagonal or only off-diagonal disorder. We have clearly demonstrated that our numerical results follow the universal behavior suggested in Ref. 12 after a suitable scaling of the DOS and energy. For the 3D diagonal case, the universality is only obeyed in a small region around the CPA band edge and breaks down for strong disorder. The 3D diagonal-disorder results show clearly

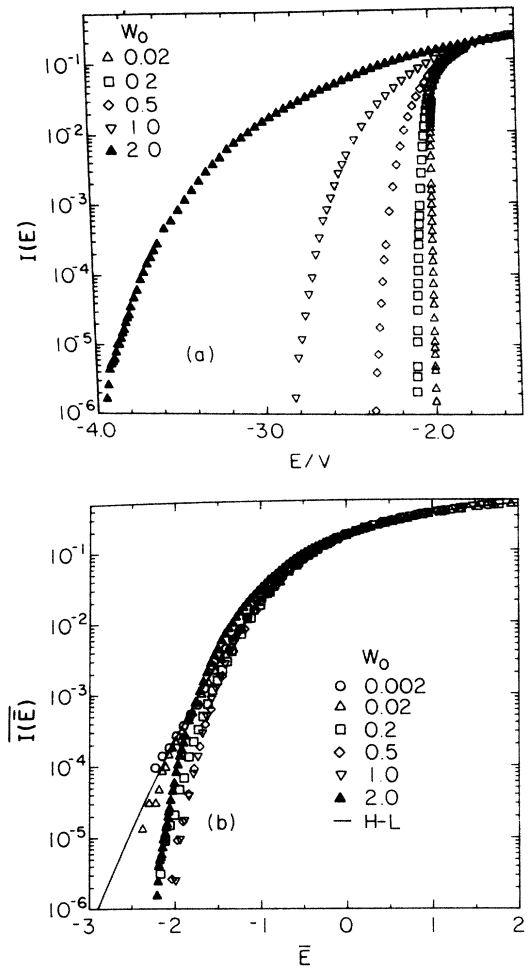

FIG. 7. (a) Plot of the tail-integrated density of states $I(E)$ as a function of energy E for the 1D tight-binding model with pure off-diagonal disorder of strength W_0. (b) Plot of the 1D scaled tail-integrated density of states $\overline{I(\bar{E})}$ as a function of the scaled energy E for pure off-diagonal disorder, $\overline{I(\bar{E})}=I(E)\times L'_{01}$, $\bar{E}=(E'-2V)/\varepsilon'_{01}$, where $\varepsilon'_{01}=w_e^{4/3}/V^{1/3}$, $L'_{01}=(V^{2/3}/w_e^{2/3})a$, and E', w_e are defined in Eqs. (2.5a)–(2.5c). The solid line is the universal curve of Halperin-Lax theory (Refs. 4 and 12). The maximum size of systems is 5×10^6.

that the behavior of the DOS is a simple exponential as a function of energy. The slope E_0 of that exponential is proportional to the square of the standard deviation of the diagonal disorder, in agreement with the CPA and path-integral–formalism predictions. For the off-diagonal case, we, for the first time, within the formulation of homomorphic cluster CPA, write down the CPA equations (the details are given in the Appendix). The main conclusion of our analytic CPA results is that to second order in w_0, i.e., weak off-diagonal disorder, the CPA equations for off-diagonal disorder in any dimension look similar to those of the diagonal-disorder case. Then by the appropriate scaling given in Eqs. (2.5a)–(2.5c), all the analytical results for the diagonal-disorder case can be also used for the off-diagonal case. We have numerically checked these ideas and given excellent results for the 1D case in agreement with previous studies.[22,24] For the 2D and 3D off-diagonal-disorder cases, we obtain results that follow the universality suggested in Ref. 12. From our numerical results for the 3D off-diagonal case, it is difficult to draw the conclusion that the DOS versus E behaves as a simple exponential. However, for the 3D diagonal case, the exponential behavior of the DOS is clearly demonstrated. In conclusion, we have demonstrated both analytically and numerically the general validity of the universal behavior particularly near band edges. For $D>1$, universality remains after a nonuniversal shift of the unperturbed band edge. We also demonstrated that a reasonable understanding of the behavior of the DOS of weakly disordered systems with diagonal or off-diagonal disorder in any dimension can be achieved by the coherent potential approximation.

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APPENDIX

The homomorphic cluster coherent-potential approximation (HCPA) condition for a two-site cluster is expressed by a matrix equation as

$$\langle \tilde{T}\rangle=\langle \tilde{v}(1-\tilde{g}\,\tilde{v})^{-1}\rangle=0\ , \tag{A1}$$

where

$$\tilde{v}=\begin{bmatrix}\alpha(\varepsilon_1-\Sigma) & V_{12}-V_\Sigma\\ V_{12}-V_\Sigma & \alpha(\varepsilon_2-\Sigma)\end{bmatrix}\ , \tag{A2}$$

$$\tilde{g}=\begin{bmatrix}g_{11} & g_{12}\\ g_{21} & g_{22}\end{bmatrix}\ . \tag{A3}$$

$1/\alpha=n$ is the number of the nearest neighbor. The effective Green's function is defined as

$$g_{ij}(Z)\equiv\langle i\,|\,(ZI-H_{\rm eff})^{-1}\,|\,j\rangle = \frac{V}{V_\Sigma}g^0_{ij}\left[\frac{V}{V_\Sigma}(Z-\Sigma)\right]\ , \tag{A4}$$

where g^0_{ij} is the unperturbed Green's function with transfer energy $V=\langle V_{12}\rangle$ and $Z=E+iS$, and the effective Hamiltonian $H_{\rm eff}$ is given as

$$H_{\rm eff}=\sum_i \Sigma\,|\,i\rangle\langle i\,|+V_\Sigma\,|\,i\rangle\langle i+1\,|+V_\Sigma\,|\,i+1\rangle\langle i\,|\ . \tag{A5}$$

ε_1 and ε_2 are random-site energies (diagonal disorder) and V_{12} is the random transfer energy (off-diagonal disorder). The coherent potential Σ and the coherent transfer energy V_Σ are determined by condition (A1).

For pure off-diagonal disorder, we take $\varepsilon_i=0$ for simplicity, and Eq. (A1) becomes

$$\langle \tilde{T} \rangle = \left\langle \frac{1}{C} \begin{bmatrix} -\alpha\Sigma - [\alpha^2\Sigma^2 - (V_{12}-V_\Sigma)^2]g_{11} & (V_{12}-V_\Sigma) + [\alpha^2\Sigma^2 - (V_{21}-V_\Sigma)^2]g_{12} \\ (V_{12}-V_\Sigma) + [\alpha^2\Sigma^2 - (V_{12}-V_\Sigma)^2]g_{12} & -\alpha\Sigma - [\alpha^2\Sigma^2 - (V_{12}-V_\Sigma)^2]g_{22} \end{bmatrix} \right\rangle = 0 . \tag{A6}$$

where

$$C \equiv 1 + 2\Sigma g_{11} - 2(V_{12}-V_\Sigma)g_{12} + (g_{11}^2 - g_{12}^2)[\alpha^2\Sigma^2 - (V_{12}-V_\Sigma)^2] \tag{A7}$$

using $g_{11}=g_{22}$ and $g_{12}=g_{21}$; Eq. (A6) can also be written as two equations:

$$\left\langle \frac{1}{C}\{-\alpha\Sigma - [\alpha^2\Sigma^2 - (V_{12}-V_\Sigma)^2]g_{11}\} \right\rangle = 0 , \tag{A8a}$$

$$\left\langle \frac{1}{C}\{V_{12}-V_\Sigma + [\alpha^2\Sigma^2 - (V_{12}-V_\Sigma)^2]g_{12}\} \right\rangle = 0 . \tag{A8b}$$

For weak disorder, we anticipate $\Sigma \sim w_0^2 V$ and $V_\Sigma - V \sim w_0^2 V$, where

$$w_0^2 = \frac{\langle (V_{12}-V)^2 \rangle}{V^2} \tag{A9}$$

represents the strength of the off-diagonal disorder. Keeping the leading terms in w_0^2, Eqs. (A8a) and (A8b) become

$$\alpha\Sigma = w_0^2 V^2 g_{11} , \tag{A10a}$$

$$V_\Sigma - V = w_0^2 V^2 g_{12} . \tag{A10b}$$

Furthermore, for a regular lattice (square in two dimensions, simple cubic in three dimensions, and simple hypercubic in general) the relation

$$2dVg_{12}^0 = -1 + Zg_{11}^0 \tag{A11}$$

holds. Hence, from Eqs. (A10a) and (A10b),

$$\begin{aligned} \frac{V_\Sigma - V}{V} = Vw_0^2 g_{12} &= Vw_0^2 \frac{V}{V_\Sigma} g_{12}^0 \left[\frac{V}{V_\Sigma}(Z-\Sigma) \right] \\ &= Vw_0^2 \frac{V}{V_\Sigma} \left[-\frac{1}{2dV} + \frac{Z-\Sigma}{2dV_\Sigma} g_{11}^0 \left[\frac{V}{V\Sigma} \right] \right] \\ &= Vw_0^2 \frac{V}{V_\Sigma} \left[-\frac{1}{2dV} + \frac{Z-\Sigma}{2dV} \frac{\alpha\Sigma}{w_0^2 V^2} \right] \\ &\simeq -\frac{w_0^2}{2d} + \frac{Z-\Sigma}{2d}\alpha\Sigma + O(w_0^4) . \end{aligned} \tag{A12}$$

Substituting Eq. (A12) into Eq. (A10a) and keeping only the leading term, w_0^2, we have

$$\begin{aligned} \alpha\Sigma = w_0^2 V^2 g_{11} &= w_0^2 V^2 \frac{V}{V_\Sigma} g_{11}^0 \left[\frac{V}{V_\Sigma}(Z-\Sigma) \right] \\ &= w_0^2 V^2 \frac{V}{V_\Sigma} g_{11}^0 \left[(Z-\Sigma) - (Z-\Sigma)\left[\frac{V_\Sigma}{V} - 1 \right] + O(w_0^4) \right] \\ &= w_0^2 V^2 g_{11}^0 \left\{ Z\left[1 + \frac{w_0^2}{2d} \right] - \left[1 + \left[\frac{Z^2\alpha}{2dV^2} \right] \right] \Sigma \right\} + O(w_0^4) . \end{aligned} \tag{A13}$$

Now let us define

$$Z' \equiv \left[1 + \frac{w_0^2}{2d} \right] Z , \tag{A14a}$$

$$\Sigma' \equiv \left[1 + \frac{Z^2\alpha}{2dV^2} \right] \Sigma , \tag{A14b}$$

$$w_e \equiv \left[\frac{1}{\alpha} + \frac{Z^2}{2dV^2} \right]^{1/2} w_0 ; \tag{A14c}$$

then, the HCPA equation (A13) can be written as

$$\Sigma' = w_e^2 g_{11}^0 (Z' - \Sigma') \ . \tag{A15}$$

This is exactly the one-site CPA condition for diagonal disorder up to $O(w^4)$. Therefore, a relation between the off-diagonal disorder HCPA and diagonal CPA is established up to $O(w^4)$. Explicitly, around the band edge $z = \pm 2dV$,

$$w_e' = 2\sqrt{d}\, w_0 = \begin{cases} 2w_0 & \text{for one dimension ,} \\ \sqrt{8}w_0 & \text{for two dimensions ,} \\ \sqrt{12}w_0 & \text{for three dimensions ,} \end{cases} \tag{A16}$$

where in Eq. (A15) $1/\alpha = n = 2d$ is used.

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[1]F. Urbach, Phys. Rev. **92**, 1324 (1953).

[2]G. D. Cody, *Semiconductors and Semimetals* (Academic, New York, 1985), Vol. 21B, p. 11.

[3]Y. Toyozawa, Prog. Theor. Phys. **20**, 53 (1958); **22**, 455 (1959); H. Sumi and Y. Toyozawa, J. Phys. Soc. Jpn. **31**, 342 (1971); S. Abe and Y. Toyozawa, *ibid.* **50**, 2785; M. Schreiber and Y. Toyozawa, *ibid.* **51**, 1528, 1537, 1544 (1982).

[4]B. I. Halperin and M. Lax, Phys. Rev. **148**, 722 (1966).

[5]I. Z. Kostadinov, J. Phys. C **10**, L263 (1977).

[6]J. Dow and D. Redfield, Phys. Rev. B **1**, 3358 (1970); J. Dow and D. Redfield, *ibid.* **5**, 514 (1972).

[7]T. Skettrup, Phys. Rev. B **18**, 2622 (1978).

[8]C. M. Soukoulis, M. H. Cohen, and E. N. Economou, Phys. Rev. Lett. **53**, 616 (1984).

[9]W. Stritrakool, V. Sa-yakanit, and H. R. Glyde, Phys. Rev. B **33**, 1199 (1986), and references therein.

[10]S. John, C. M. Soukoulis, M. H. Cohen, and E. N. Economou, Phys. Rev. Lett. **57**, 1777 (1986); M. Y. Chou, S. John, M. H. Cohen, and C. M. Soukoulis (unpublished).

[11]D. Monroe and M. A. Kastner, Phys. Rev. B **33**, 8881 (1986).

[12]E. N. Economou, C. M. Soukoulis, M. H. Cohen, and A. D. Zdetsis, Phys. Rev. B **31**, 6172 (1985); C. M. Soukoulis, A. D. Zdetsis, and E. N. Economou, *ibid.* **34**, 2533 (1986).

[13]M. H. Cohen, E. N. Economou, and C. M. Soukoulis, Phys. Rev. **32**, 8268 (1985).

[14]E. N. Economou, C. M. Soukoulis, M. H. Cohen, and S. John, in *Disordered Semiconductors,* edited by M. Kastner (Plenum, New York, 1987), p. 681; N. Bacalis, E. N. Economou, and M. H. Cohen (unpublished).

[15]E. Brezin and G. Parisi, J. Phys. C **13**, L307 (1980); J. L. Cardy, *ibid.* **11**, L321 (1978).

[16]D. J. Thouless and M. E. Elzain, J. Phys. C **11**, 3425 (1978).

[17]Z-Q. Zhang and P. Sheng, Phys. Rev. Lett. **57**, 909 (1987).

[18]P. Dean, Rev. Mod. Phys. **44**, 127 (1972).

[19]C. M. Soukoulis and E. N. Economou, Phys. Rev. B **24**, 5698 (1981).

[20]E. N. Economou, *Green's Functions in Quantum Physics,* 2nd ed. (Springer, Heidelberg, 1983), Chap. 7.

[21]F. Yonezawa and T. Odagaki, J. Phys. Soc. Jpn. **47**, 388 (1977).

[22]A. Mieke and F. Wegner, Z. Phys. B **62**, 1 (1985).

[23]B. Derrida and E. Gardner, J. Phys. (Paris) **45**, 1283 (1984).

[24]S. N. Evangelou, J. Phys. C **20**, L89 (1987).

[25]*The Recursion Method and its Applications,* Vol. 58 of *Springer Tracts in Modern Physics,* edited by D. G. Pettifor and D. L. Weaire (Springer, Berlin, 1985).

[26]S. N. Evangelou, J. Phys. C **19**, 4291 (1987), and references therein.