Localization in three-dimensional systems by a Gaussian random potential

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The electronic localization properties of a three-dimensional (3D) cubic system under the influence of a random potential having a Gaussian probability distribution are studied by the potential-well-analogy method. The results are compared with the localization-function method as well as with numerical results using the strip method. The overall shape and size of the mobility-edge trajectory is found to be significantly different than the one obtained using a rectangular distribution for the random potential. In contrast to the case of the rectangular distribution for the random potential, where the mobility edge at the band center was located at $W=16.5$ V, the corresponding effective W_c for the Gaussian distribution is found at $W_c=21.5$ V. We have confirmed this prediction by performing numerical calculations using one-parameter scaling in 3D strips.

I. INTRODUCTION

Over the last two years, the concept of the potential-well analogy (PWA) has been developed and applied very successfully[1-4] to the problem of electronic localization, especially in connection with simple mean-field theories such as the coherent-potential approximation (CPA). Through the application of the PWA method, which exploits a mathematical equivalence between the localized states in disordered systems and the bound states in local-potential wells, very useful results and fruitful ideas have emerged.[2-5] A good example of such an idea which also explains the success of the PWA method is the concept of universality in certain basic features of disordered systems for low disorder and near the band edges.[2-5] This universality is brought up by introducing natural units of length and energy and by forming proper dimensionless quantities using these natural units.

We have chosen to examine in more detail the application of the PWA in a three-dimensional (3D) system using a Gaussian distribution for the random potential. The introduction of a Gaussian distribution is very interesting on its own merit because of the exponential tails which appear in the density of states as a result of the tails in the random potential.[4,5] It can also be used to check the ideas of the universality as well as the sensitivity, if any, of the trajectory of the mobility edge on the type of the probability distribution.[6]

In Sec. II we briefly describe 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

The tight-binding Hamiltonian which describes the system including only diagonal disorder is of the form

$$H=\sum_n |n\rangle\varepsilon_n\langle n| + V\sum_{n,m}{}' |n\rangle\langle m| \ , \tag{2.1}$$

where the sites (n) form a regular cubic lattice, V is the hopping matrix element, and $p(\varepsilon_n)$ is the common probability distribution of each site energy. We can distinguish two main classes of $p(\varepsilon_n)$: (i) the terminating ones, such as the rectangular distribution, considered in our previous work, of total width W and variance $w^2=W^2/12$, for which $p(\varepsilon_n)=0$ when $|\varepsilon_n| \gg w$, and (ii) the ones with tails, such as the Gaussian distribution which we will consider here,

$$p(\varepsilon_n)=\frac{1}{\sqrt{2\pi}w}\exp\left[-\frac{\varepsilon_n^2}{2w^2}\right] , \tag{2.2}$$

for which $p(\varepsilon_n)\neq 0$ even when $|\varepsilon_n| \gg w$.

The CPA calculates the average Green's function G corresponding to H from an effective periodic Hamiltonian resulting from (2.1), by replacing ε_n by a common self-energy Σ, which is determined by a self-consistent equation.[1,4,7] By this procedure, the self-energy, the Green's function, the mean-free-path length, $l(E)$, the conductivity[1,4,7] $\sigma_0(E)$ and the constant-energy surface $S(E)$ in 3D, are calculated. The details of this procedure can be found in Refs. 1, 4, and 7. However, the CPA, being a mean-field theory, omits certain fluctuations which are responsible for important physical effects, such as the localization of some eigenstates and the strong amplitude fluctuations of some other extended states.

It has been pointed out recently that this omission can be remedied, so far as the localized states are concerned, by considering the most elementary problem in quantum mechanics, that of a bound state in a shallow effective-potential well. The depth V_0 of the effective-potential well is proportional to $\sigma_0(E)^{-1}l(E)^{-D}$, where D is the dimensionality and the width α is proportional to $l(E)$. As we mentioned above, by employing the CPA one can find at every energy E the mean free path $l(E)$ and the CPA conductivity $\sigma_0(E)$; then from $l(E)$ and $\sigma_0(E)$ one can construct the effective-potential well characterized by $\alpha(E)$ and $V_0(E)$. If this potential well can sustain a bound state with a decay length $\lambda(E)$ then the eigenstates at E are localized with localization length $\lambda(E)$. If no bound state exists at the effective-potential well, the eigen-

states of E are extended. In three dimensions, the mobility-edge energy E_c, which separates extended-form localized states is given by the relation[1,4]

$$S(E_c)l^2(E_c)=8.96\ . \tag{2.3}$$

It is important to stress that quantities obtained from the approximate scheme outlined above (based on the CPA and the potential-well analogy) are in satisfactory agreement[1,4,8,9] with results based on independent numerical methods.

III. RESULTS AND DISCUSSION

We show in Fig. 1 the density of states (DOS) for three different w. In the same figure for a comparison we also plot the corresponding DOS for rectangular distributions of the same variance, i.e., of total width $W=w\sqrt{12}$. The long tails present in the DOS of the Gaussian probability distributions, as mentioned earlier, are due to the fact that contrary to the rectangular distributions there is always a finite (but very small) probability for a very deep fluctuation of some ε_n, while the neighboring ε_n have values in the range $(-w,w)$. Such an isolated potential well can trap an electron around it. It should be mentioned that the CPA,[1,4,7] which treats rigorously the scattering from a single site, correctly describes the extreme tail in the DOS resulting from these single-site bound states. In Fig. 1 we have also marked the CPA band edges as defined by the approximate equation[4]

$$E_{\mathrm{CPA}}/V=6+0.253\frac{w^2}{V^2}-\left[\frac{1}{64\pi^2}+(0.253)^3a\right]\frac{w^4}{V^4}\ , \tag{3.1}$$

where $a=\frac{1}{5}$ for the rectangular distribution, and -1 for the Gaussian. This equation is obtained by combining the asymptotic expansion of self-energy Σ valid for low disorder[4] ($wG\ll 1$),

$$\Sigma=w^2G-(2w^4-\mu_4)G^3+O(w^6) \tag{3.2}$$

with appropriate expansions of G near the band edges. In the above relation (3.2), μ_4 is the fourth moment of the distribution $p(\varepsilon_n)$ and is equal to $9w^4/5$ for the rectangular and $3w^4$ for the Gaussian distribution. This approximate CPA equation (3.2), contrary to the full CPA equation[4] cannot describe the deep-tail states, which are associated with the pole of the integrand[4] appearing in the CPA for the self-energy Σ. Thus it is expected that E_{CPA} in the Gaussian case simply separates the deep-tail states from the band states. For the rectangular distribution, as can be seen in Fig. 1, the meaning of E_{CPA} is quite obvious; it marks the CPA band edge beyond which the CPA DOS drops to zero. Furthermore, for low disorder, the approximate Eq. (3.1) is in very good agreement with the results of the numerical solution of the CPA equation [see Figs. 1(a) and (1b)]. For the Gaussian distribution, however, E_{CPA} defines a crossover energy at which the behavior of the DOS changes from algebraic "bandlike" to an exponential tail [see, e.g., Fig. 2(b)]. For large disorder the bandlike DOS approaches that of the probability distribution of ε_n. Note that E_{CPA} is a nonuniversal[4] and

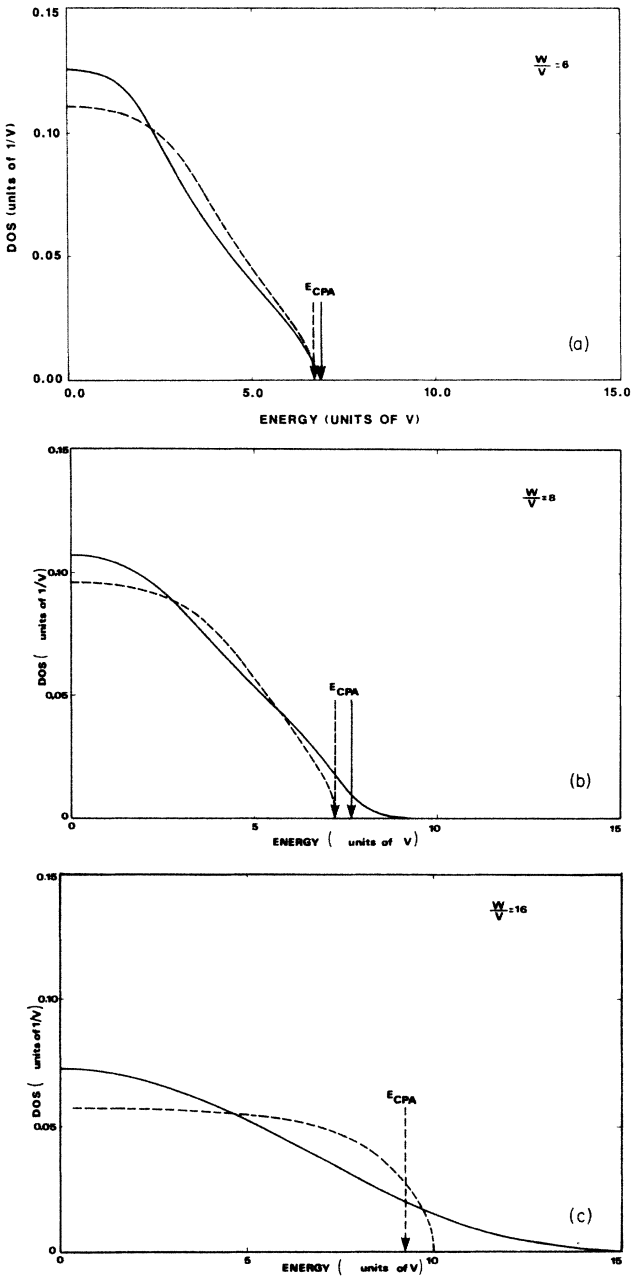

FIG. 1. CPA density of states for Gaussian (solid line) and rectangular (dashed line) distributions of the same variance $w^2=W^2/12$ for three different disorders: (a) for $W=6V$, (b) for $W=8V$, and (c) for $W=16V$. The corresponding arrows, solid and broken, indicate the CPA band edges as defined by the approximate Eq. (3.1) for the Gaussian and rectangular distribution, respectively. In (c) the arrow corresponding to the Gaussian band edge is located at $19V$ off the figure frame.

depends on the particular lattice structure and probability distribution.[4] It serves, though, to define universal quantities, once energies are measured from it and proper energy units are used.[4,5] In Fig. 1(c) we can see that E_{CPA} as obtained by Eq. (3.1) differs appreciably from the corresponding numerical value for the rectangular case and it has particular meaning for the Gaussian case. This was expected for such a large disorder ($w=4.62V$ or $W=16V$). To further illustrate the nature of the tails in

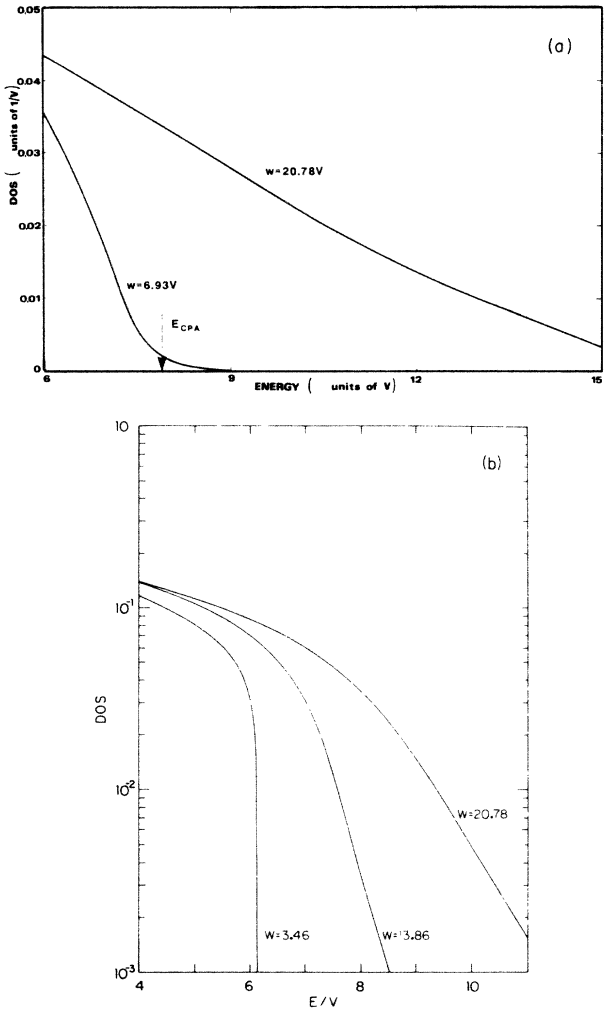

FIG. 2. (a) CPA tails of the DOS for Gaussian distribution and for $w=2V$ (i.e., $W=\sqrt{12}w=6.93V$) and $w=6V$ (i.e., $W=\sqrt{12}w\simeq 20.78V$). The arrow indicates the CPA band edge defined by Eq. (3.1). The logarithmic scale of (b) demonstrates the approximate exponential nature of the trial. Notice that in (b) $w=1V$ (i.e., $W=3.46V$), $w=4V$ (i.e., $W=13.86V$) and $W=6V$ (i.e., $W=20.78V$).

the DOS, we plot in Fig. 2(a) the DOS for $w=2V,6V$ (or $W=6.93V,20.78V$, respectively) in the range $E=6V$ to $E=15V$. It can be verified here as was shown before that these deep tails display exponential behavior of the form $\exp(-E/E_0)$, where E_0 depends approximately linearly on the second power of the disorder

$$E_0=c\frac{w^2}{V} . \tag{3.3}$$

This is clearly shown in Fig. 2(b) where the logarithm of DOS versus E/V is plotted for different values of w. The value of c predicted analytically on the basis of an asymptotic equation[4] and valid for medium disorder, is $c\simeq 0.12$. We found c close to the analytic asymptotic value but slightly w dependent as shown in Fig. 3 in agreement with Abe-Toyozawa.[10] The small differences about the correct value of c between this work and Abe and Toyozawa's are due to the different unperturbed Green's functions that were used. Abe and Toyozawa[10] used the Hubbard density of states,[7] while in this work the density of states for a cubic lattice is used. The results for the Hubbard density of states, shown in Fig. 3, were generated by us and agree with that for Ref. 10.

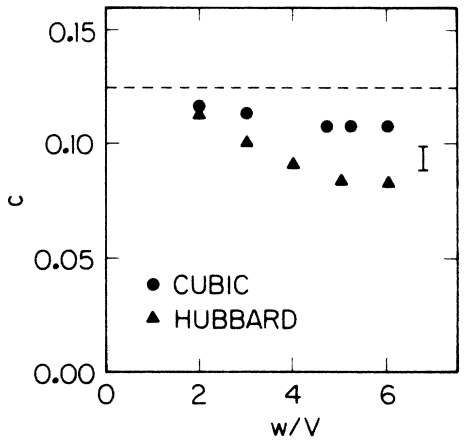

FIG. 3. Variation of the "constant" c (Eq. 3.3) with disorder w ($w=W/\sqrt{12}$) for cubic lattice and Hubbard model. The size of the error bar is due to uncertainties of fitting the logarithm of DOS to E/E_0, where E_0 is given by cw^2/V.

The CPA band edge $E_{\rm CPA}$, as was defined by Eqs. (3.1) and (2.1), can also be used for lower disorder to obtain analytically the mobility edge E_c which separates extended from localized states.[4] The relation between the two is given by[4]

$$E_c-E_{\rm CPA}\simeq -2.852\frac{w^4}{4(4\pi)^2V^3} , \tag{3.4a}$$

or

$$E_c-E_{\rm CPA}\simeq -4.515\times 10^{-3}\left[\frac{w}{V}\right]^4 V . \tag{3.4b}$$

From Eqs. (3.4a) and (3.1), it is obvious that (i) for low disorder E_c is outside the unperturbed band edge which is given by $6V$, and (ii) E_c is further out from the unperturbed band edge for the Gaussian than for the rectangular distribution, since, as is also shown in Figs. 1(a)–1(c), the corresponding CPA band edge for the Gaussian distribution is further away than the one for the rectangular distribution. Both of these conclusions are in strong disagreement with the recent work of Schreiber[6] who finds E_c inside the unperturbed band edges, for all w's.

In a very recent publication,[8] using a rectangular probability distribution we have checked against numerical data not only Eqs. (3.4a) and (3.4b), but the complete mobility-edge trajectory obtained by the numerical solution of Eq. (2.1) combined with the CPA. The agreement between the numerical results and our approximation was impressive. We have recalculated here, using the Gaussian probability distribution, the complete mobility-edge trajectory. The results are plotted in Fig. 4 together with the trajectory for the rectangular based on the PWA and the trajectory for Gaussian calculated by the localization-function technique.[11] The localization function we have used here has the form[11,1]

$$L(E)=KVt^{1/3} , \tag{3.5a}$$

with $K=4.6862$,

$$t=D/G_0 , \tag{3.5b}$$

and

$$D=\{[G_0+G_0(1,1,0)]^2-4G_0^2(1,0,0)\} \times[G_0-G_0(1,1,1)]^2 . \tag{3.5c}$$

The arguments of all diagonal and nondiagonal matrix elements of the Green's functions above are $E-\Sigma(E)$. From Fig. 4 we have the following observations.

(a) The shape of the trajectory in Fig. 4, especially the upper part corresponding to higher disorder, is quite different from the one obtained with the rectangular distribution[1,8] whereas the lower parts, corresponding to lower disorders, are almost the same. This is to be expected, because for small disorder the difference in $E_{\rm CPA}$ and E_c [Eqs. (3.1) and (3.4a)] between Gaussian and rectangular distribution is very small.

(b) Our results are in disagreement with those of Schreiber,[6] in that our trajectory, as was expected from (3.4a), is outside the unperturbed band edges for low up to moderate ($W\sim 11V$) disorders and that the corresponding critical disorder at the band center that we find here is $W_c/V=21.5\pm0.5$ compared to 16.4 ± 0.3 in Schreiber's work.[6] However, the general shape of our trajectory for Gaussian distribution and large disorder starting at $W=6V$, apart from a scale factor is similar to Schreiber's.

(c) The PWA and the localization-function techniques give results in very good agreement for low and moderate (up to $W\sim 15V$) disorder. For disorder larger than $W=16V$, the PWA and localization-function trajectories are different in magnitude but similar in shape. Since the PWA results agree well with the numerical data, as will be explained below, it follows that the $L(E)$ method underestimates the critical disorder for $E=0$ by about 23%, while for the rectangular case the corresponding underestimation is about 13%. The reasons for this underestimation are not clear.

For very large disorder the DOS takes the shape of one probability distribution [see for example Fig. 1(c)]. Therefore, near the band center one qualitatively expects that the Gaussian probability distribution will give higher DOS and higher mobility-edge trajectory than the rectangular probability distribution. We can see this more clearly by combining the approximate relation for large disorder ($w\to\infty$) for the self-energy Σ and Green's function G at the center of the band $E=0$ with Eq. (2.3). For the $w\to\infty$ limit we have that[1]

$$\mathrm{Im}\Sigma(0)=\frac{1}{\pi p(0)} , \tag{3.6a}$$

$$G(0)=-i\pi p(0) , \tag{3.6b}$$

where $p(0)$ is the random probability distribution for $E=0$. [$p(0)=1/W$ and $1/w\sqrt{2\pi}$ for the rectangular and Gaussian probability, respectively.] In the $w\to\infty$ limit, $\Sigma(E)=1/G(E)$. Since $l=v\tau$, $\tau=\hbar/2\Sigma_2$, $\Sigma_2=\mathrm{Im}\Sigma(E)$, and using Eq. (2.3) we obtain that the ratio of the critical disorder $W_{\rm cr}(0)$ for the rectangular distribution over the same quantity for the Gaussian distribution $W_{\rm CG}(0)$ is equal to $(2\pi/12)^{1/2}=0.72$. This is in good agreement with our results which give $W_{cr}(0)=16.5$ and $W_{\rm CG}(0)=21.5V$.

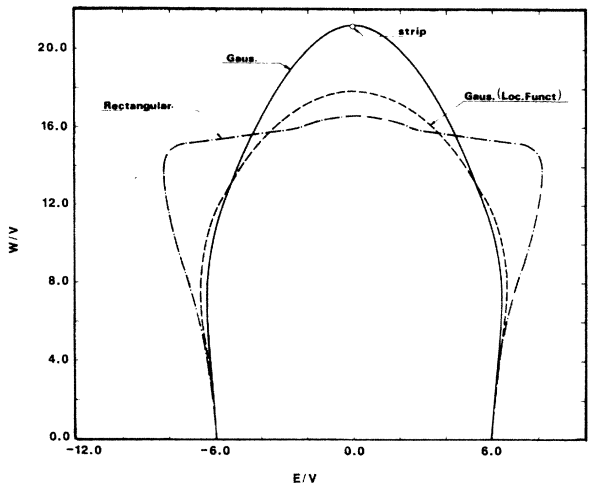

FIG. 4. Mobility-edge trajectory for Gaussian distribution with the PWA method (solid line) and the localization function method (dashed line) together with the mobility-edge trajectory, for the rectangular distribution obtained with the PWA method (broken line). W is the corresponding width of the rectangular distribution with the same variance. The open circle indicates the numerical result of the strip or wire method.[12–15]

To further check these results beyond the CPA-PWA regime, we have resorted to finite-size-scaling methods using the very reliable technique of strip or wire.[8,12–15] In this method, one considers coupled one-dimensional systems. Each one-dimensional system is described by tight-binding Hamiltonian of the form (2.1). The coupling of the chains, placed together to form a cylinder of square cross section, is characterized by an interchain matrix element. As the number of coupled chains approaches infinity we recover the three-dimensional system. The common probability distribution $p(\varepsilon_n)$ for each one-dimensional system contrary to earlier work is taken as a Gaussian of width w. For the M regularly placed chains of length N, one determines the largest localization length λ_M as $N\to\infty$. Then from a plot of λ_M versus M one can determine the localization properties of the system.[12–15] In particular by studying λ_M/M versus M one obtains a reasonable estimate of the mobility edge. At exactly the mobility edge[12–15] $\lambda_M/M=0.6$ while for extended and localized states we have λ_M/M versus M increases and decreases, respectively. In Table I we have listed λ_M versus M for $M=2,3,4,5,6$ for two representative values of $w/V=6,7$. We have found, as is also indicated in Table I, that the critical disorder at the band center is $w_c/V=6\pm0.25$ with an effective width W of the corresponding rectangular distribution $W_c/V=21\pm1$, in very good agreement with our PWA results.

IV. CONCLUSIONS

This paper demonstrates that the potential-well analogy coupled with the CPA is capable of producing results not only in qualitative but in quantitative agreement with in-

TABLE I. Selective numerical results at $E=0$ strip and wire method.

$E=0$	$w=6.0$		$w=7.0$	
M	λ_M	λ_M/M	λ_M	λ_M/M
2	1.2445	0.62	1.0639	0.53
3	1.8008	0.60	1.4803	0.49
4	2.3209	0.58	1.8437	0.46
5	2.9682	0.59	2.2536	0.44
6	3.5315	0.59	2.5914	0.42

dependent numerical data. For a 3D-tight-binding model with a Gaussian probability distribution we obtain the dependence of the mobility edge on the strength of the diagonal disorder. For large disorder the shape of the mobility-edge trajectory depends on the probability distribution. For Gaussian probability distribution we find that the critical disorder at the band center is 21.5 and the shape of the mobility-edge trajectory reflects the Gaussian nature of the probability distribution. On the other hand, for the rectangular probability distribution,[8] we obtain 16.5 as the value of the critical disorder at the band center and the shape of the mobility-edge trajectory is flat for large W, reflecting the nature of the rectangular distribution. For values of disorder up to $W=10$ we have that the mobility-edge trajectory is almost the same for the rectangular and Gaussian probability distribution. Our results have been verified independently by numerical data based on the one-parameter scaling strip or wire method.[12–15] The discrepancies, about the shape of the mobility-edge trajectory and the critical value of disorder at $E=0$ for the Gaussian probability distribution, between this work and the work of Schreiber[6] are most probably due to the numerical uncertainties in his calculations. He used small sized systems, ($7\times5\times5$ and $12\times10\times9$).

Finally, we have verified that the Gaussian probability distribution[16] within the CPA produces long exponential tails[4] of the form $\exp(-E/E_0)$ with $E_0=cw^2/V$ with c slightly w dependent ($c\simeq0.11$), but in qualitative agreement with Abe-Toyozawa.[10] The small differences are due to the different unperturbed Green's functions used. Abe and Toyozawa[10] used the Hubbard density of states, while in this work the density of states for a cubic lattice is employed.

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[1]E. N. Economou and C. M. Soukoulis, Phys. Rev. B **28**, 1093 (1983); E. N. Economou, C. M. Soukoulis, and A. D. Zdetsis, *ibid.* **30**, 1686 (1984).

[2]E. N. Economou, Phys. Rev. B **31**, 7710 (1985).

[3]E. N. Economou, C. M. Soukoulis, and A. D. Zdetsis, Phys. Rev. B **31**, 6483 (1985).

[4]E. N. Economou, C. M. Soukoulis, M. H. Cohen, and A. D. Zdetsis, Phys. Rev. B **31**, 6172 (1985).

[5]C. M. Soukoulis, M. H. Cohen, E. N. Economou, and A. D. Zdetsis, J. Non-Cryst. Solids **77/78**, 47 (1985); E. N. Economou, A. D. Zdetsis, and D. A. Papaconstantopoulos, *ibid.* **77/78**, 147 (1985).

[6]M. Schreiber, Phys. Rev. B **31**, 6146 (1985).

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

[8]A. D. Zdetsis, C. M. Soukoulis, and E. N. Economou, and G. S. Grest, Phys. Rev. B **32**, 8711 (1985).

[9]A. D. Zdetsis, in *Hydrogen in Disordered and Amorphous Solids,* edited by G. Bambakidis and R. C. Bowman (Plenum, New York, 1986); E. N. Economou, C. M. Soukoulis, and M. H. Cohen, *ibid.*

[10]S. Abe and Y. Toyozawa, J. Phys. Soc. Jpn. **50**, 2185 (1981).

[11]D. C. Licciardello and E. N. Economou, Phys. Rev. B **11**, 3697 (1975).

[12]J. L. Pichard and G. Sarma, J. Phys. C **14**, L127 (1981).

[13]A. MacKinnon and B. Kramer, Phys. Rev. Lett. **47**, 1546 (1981); **49**, 695 (1982); Z. Phys. B **53**, 1 (1983).

[14]C. M. Soukoulis, I. Webman, G. S. Grest, and E. N. Economou, Phys. Rev. B **26**, 1838 (1982).

[15]E. Abrahams, P. W. Anderson, D. C. Licciardello, and T. V. Ramakrishnan, Phys. Rev. Lett. **42**, 673 (1979).

[16]B. I. Halperin and M. Lax, Phys. Rev. **153**, 802 (1967).