Localized states in disordered systems as bound states in potential wells

E. N. Economou* and C. M. Soukoulis†
Corporate Research Science Laboratory, Exxon Research and Engineering Company, Annandale, New Jersey 08801

A. D. Zdetsis
Department of Physics, University of Crete and Research Center of Crete, Heraklio, Crete, Greece
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The equivalence between localized states in disordered d-dimensional systems and bound states in local potential wells (or local potential fluctuations) in d-dimensional space is tested against numerical data. The agreement is found to be satisfactory. A new criterion for the onset of localization is deduced. It reduces to Mott's criterion at the center of the band but it differs qualitatively from Mott's picture when the mobility edge is near the band edges.

I. INTRODUCTION

It has been suggested recently[1,2] that there is a mathematical connection between the problem of localization in disordered systems and the elementary problem of bound states in potential wells. The argument supporting this suggestion can be summarized as follows. The $T=0$ configurationally averaged conductivity σ, which is proportional to $\langle \mathrm{Tr}(\hat{p}\hat{G}_2\hat{p}\hat{G}_2)\rangle$, is usually approximated by $\mathrm{Tr}(\hat{p}\langle\hat{G}_2\rangle\hat{p}\langle\hat{G}_2\rangle)$ to produce the well-known expression[2]

$$\sigma \approx \sigma_0 = \frac{2e^2\hbar}{\pi\Omega d}\sum_{\vec{k}} v^2(\vec{k})\langle G_2(E,\vec{k})\rangle^2 . \tag{1.1}$$

$\hat{G}_2(E)$ is the imaginary part of the Green's function $\hat{G}(E)=(E-\hat{H})^{-1}$, $\hat{p}$ is the momentum operator, d is the dimensionality, Ω is the volume of the specimen, and $\vec{v}(\vec{k})=\partial E(\vec{k})/\hbar\partial\vec{k}$ is the velocity. Cubic symmetry was assumed in obtaining (1.1). The next step is to identify a series of terms which were neglected by the approximation $\langle\hat{G}_2\hat{p}\hat{G}_2\rangle \approx \langle\hat{G}_2\rangle p\langle\hat{G}_2\rangle$. These terms,[3] known as maximally crossed diagrams, produce a correction to σ_0 of the following form:[2]

$$\delta\sigma \approx \sigma-\sigma_0 = -\frac{e^2}{\pi\hbar}\frac{2}{(2\pi)^d}\int d\vec{k}\frac{1}{k^2-i\omega/D_0} , \tag{1.2}$$

where $D_0=\sigma_0/2e^2\rho$ is the diffusion coefficient, ρ is the density of states (DOS) per unit cell per spin, and the limit $\omega\to 0$ must be taken. Vollhardt and Wölfle[4] made the further step to replace D_0 in the right-hand side (rhs) of (1.2) by $D=\sigma/2e^2\rho$, producing thus a self-consistent equation for σ in terms of σ_0; furthermore, they suggested[4] that in the localized regime $-i\omega/D(\omega)$ approaches λ^{-2} as $\omega\to 0^+$, where λ is the localization length. Making this replacement in (1.2) and taking into account that $\sigma(\omega)\to 0$ as $\omega\to 0$, one obtains an equation for λ in terms of σ_0. Economou and Soukoulis[1] pointed out that this equation has exactly the same structure as the equation which determines the decay length of an eigenstate bound to a potential well. The importance of this observation is that it allows one to bypass the rather complicated formalism on which localization theory is based and to reduce the localization problem to the most basic and elementary problem in quantum mechanics: that of a bound state in a potential well.

Based on the potential-well analogy one can derive immediately some basic results of localization theory: Since a weak potential well *always* binds a quantum particle in d dimensions,[2] where $d\le 2$, it follows that all eigenstates are localized in disordered d-dimensional systems for $d\le 2$. The $d=2$ system is a borderline case producing an exponentially long localization length.[2] For $d>2$ a critical strength must be exceeded (corresponding to a critical disorder for each given energy) in order to produce a bound (i.e., a localized) state. The critical exponent ν [where $\lambda\sim(\epsilon-\epsilon_c)^{-\nu}$, ϵ is the strength of the potential well, and ϵ_c is its critical value] predicted by the potential-well analogy[5] is also in agreement with the results of scaling and field theory[6] approaches to localization. Similar conclusions have been reached in Ref. 4 and in a recent paper by Kotov and Sadovskii.[7]

In the present paper we test the potential-well analogy in a quantitative way against numerical data in one dimension (1D) and two dimensions (2D). We compare also with some 3D data, although uncertainties there make the test less conclusive. In this connection we mention that Kotov and Sadovskii[7] have checked Vollhardt and Wölfle's approach[4] (which is essentially equivalent to the potential-well analogy) against data for the critical disorder needed to produce an Anderson transition in a simple cubic tight-binding model. Their results are not inconsistent with the data.

II. POTENTIAL WELLS IN TIGHT-BINDING SYSTEMS

In this section we remind the reader of the basic results concerning bound states in potential wells. We consider potential wells not in the continuum but in the less familiar but more convenient periodic tightbinding model characterized by an unperturbed Hamiltonian $\hat{H}_0$ given by

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$$\hat{H}_0 = -t \sum_{\vec{n},\vec{m}}{}' \, |\vec{n}\rangle\langle\vec{m}| , \quad t>0 \tag{2.1}$$

where the sites $\{\vec{n}\}$ form a regular lattice (square in 2D and simple cubic in 3D), of lattice constant a. The simplest potential well corresponds to adding a perturbation part H_1 to the Hamiltonian H_0, where

$$\hat{H}_1 = -\epsilon\,|0\rangle\langle 0| , \quad \epsilon>0 . \tag{2.2}$$

We consider also a slightly more complicated perturbation corresponding to a local fluctuation (rather than a local potential well) and given by

$$\hat{H}_2 = -\epsilon'\,|0\rangle\langle 0| + \epsilon'\,|1\rangle\langle 1| , \quad \epsilon'>0 \tag{2.3}$$

where the sites 0 and 1 are nearest neighbors. Both $\hat{H}_1$ and $\hat{H}_2$ produce very similar although not identical results. Overall it seems that the $\hat{H}_2$ analogy can better fit the numerical data. It is also more appealing on physical grounds since it is more natural to connect a random potential with a local fluctuation rather than a local potential well.

The energy E_{b1} of the bound level, if any, in the $\hat{H}_1$ well is given by

$$G_0(E_{b1}) = -\frac{1}{\epsilon} , \tag{2.4}$$

while that in the $\hat{H}_2$ perturbation is determined by the equation

$$G_0^2(E_{b2}) - g_0^2(E_{b2}) = \frac{1}{\epsilon'^2} . \tag{2.5}$$

In the above equations $G_0(E)$ is the diagonal matrix element of the Green's function $G_0(E) = \langle n\,|(E-\hat{H}_0)^{-1}|\,n\rangle$ and $g_0(E)$ is the nearest-neighbor off-diagonal matrix element $g_0(E) = \langle 0\,|(E-\hat{H}_0)^{-1}|\,1\rangle$. Explicit forms for the functions $G_0(E)$ and $g_0(E)$ are given in Ref. 2. The localization length λ of the bound level can be obtained as follows:[2]

$$\lambda/a = -\lim_{|\vec{m}-\vec{n}|\to\infty} \left\langle \left[\frac{1}{|\vec{m}-\vec{n}|} \ln|G_0(\vec{n},\vec{m};E_{bi})| \right]^{-1} \right\rangle_{(\vec{m}-\vec{n})/|\vec{m}-\vec{n}|} , \tag{2.6}$$

where $G_0(\vec{n},\vec{m};E_{bi}) = \langle\vec{n}\,|(E_{bi}-\hat{H}_0)^{-1}|\,\vec{m}\rangle$ and $\langle\cdots\rangle_{(\vec{m}-\vec{n})/|\vec{m}-\vec{n}|}$ denotes an average over all directions of the vector $\vec{n}-\vec{m}$. In the 1D case Eq. (2.6) becomes

$$a\lambda^{-1} = -\ln\left|\,|E_{bi}|/2t - [(E_{bi}/2t)^2-1]^{1/2}\right| . \tag{2.7}$$

In all dimensionalities and for $|E_{bi}| - Zt \ll Zt$, Eq. (2.6) reduces to the much simpler form

$$a\lambda^{-1} \approx (|E_{bi}|/t - Z)^{1/2} , \tag{2.8}$$

where Z is the coordination number ($Z=2d$). For $d=2,3$, Eq. (2.8) is adequate for all practical purposes, while for $d=1$ one can use the exact Eq. (2.7). Thus the determination of λ requires two inputs: the ratio t/ϵ (or t^2/ϵ'^2), from which E_{bi}/t can be obtained [Eqs. (2.4) and (2.5)], and the lattice spacing a, which enters in Eqs. (2.7) and (2.8).

III. RULES OF CORRESPONDENCE

In order to utilize the simple formalism for bound states in potential wells, we must express the parameters t/ϵ (or t^2/ϵ'^2) and a in terms of quantities associated with the random system under consideration. It has already been pointed out[1] that

$$\frac{Zt}{a^{d-2}|\epsilon|} = \frac{\pi\hbar d}{e^2}\sigma_0 , \tag{3.1}$$

where σ_0 is given by Eq. (1.1). In the weak scattering limit the conductivity σ_0 is given by

$$\sigma_0(E) = \frac{2}{(2\pi)^d d}\frac{e^2}{\hbar} l(E) S(E) , \tag{3.2}$$

where l is the mean free path averaged over the Fermi surface S (Fermi line for $d=2$; $S=2$ for $d=1$). Substituting Eq. (3.2) into (3.1) we obtain

$$\frac{Zt}{a^{d-2}|\epsilon|} = \frac{1}{(2\pi)^{d-1}} lS . \tag{3.3}$$

The correspondence for the $\hat{H}_2$ case and for $d=1,2$ is again determined by the requirement that in the weak limit the bound state in $\hat{H}_2$ has the same localization length as in the corresponding disordered case:

$$\frac{(Zt)^2}{a^{d-2}\epsilon'^2} = \frac{2}{(2\pi)^{d-1}} lS, \quad d=1,2 . \tag{3.4}$$

The $d=3$ rule for ϵ'^2 is such as to produce the same critical value as the single potential well, i.e.,

$$\frac{(Zt)^2}{a\epsilon'^2} = \frac{1.340\,537}{(2\pi)^2} lS, \quad d=3 . \tag{3.5}$$

The parameter a, which corresponds to the inverse of the upper cutoff in Eq. (1.2), has been assumed to be proportional to the mean free path l.[8,2] On the other hand, it has been argued[7,9] that the upper cutoff in Eq. (1.2), k_0, is equal to $x_0 k$, where k is the Fermi momentum and x_0 is expected to be between 1 and 2. The data in 2D are inconsistent with the choice $k_0 = x_0 k$ ($1<x_0<2$), while they are consistent with the choice

$$k_0 = x_0 \frac{1}{l} \tag{3.6}$$

with x_0 roughly equal to 1. Thus for the purposes of the present work we adopt Eq. (3.6) although we feel that further numerical work in 2D and 3D disordered systems is required in order to clarify the issue of the cutoff k_0. By considering the limit $E_b \to -Zt$ one can connect the cutoff k_0 with a as follows:

$$a=\left[\frac{8l}{\pi k_0}\right]^{1/2} \quad (1\text{D}) \tag{3.7a}$$

$$=\frac{8}{k_0} \quad (2\text{D}) \tag{3.7b}$$

$$=\frac{4.9887}{k_0} \quad (3\text{D})\ . \tag{3.7c}$$

IV. CALCULATION OF MEAN FREE PATH IN DISORDERED SYSTEMS

The disordered systems we consider here are Anderson's model, i.e., tight-binding models of the form

$$\hat{\mathscr{H}}=\sum_{\vec{n}} |\vec{n}\rangle\epsilon_{\vec{n}}\langle\vec{n}| - V\sum_{\vec{m},\vec{n}}{}' |\vec{n}\rangle\langle\vec{m}|\ , \tag{4.1}$$

where each $\epsilon_{\vec{n}}$ is an independent random variable with a rectangular probability distribution of total width W centered at zero. The second summation in Eq. (4.1) is over all nearest-neighbor ordered pairs. The sites $\vec{n}$ form a regular lattice (simple cubic in 3D and square in 2D). The lattice constant is taken equal to 1. The calculation of the average Green's function $\langle\hat{\mathscr{G}}(E)\rangle=\langle(E-\hat{\mathscr{H}})^{-1}\rangle$ proceeds by replacing $\hat{\mathscr{H}}$ by an effective Hamiltonian where each $\epsilon_{\vec{n}}$ has been replaced by a complex self-energy $\Sigma(E)$. According to the coherent-potential approximation (CPA)[10,2] the self-energy $\Sigma(E)$ is given by

$$\Sigma(E)=\left\langle\frac{\epsilon_{\vec{n}}}{1-(\epsilon_{\vec{n}}-\Sigma)\mathscr{G}_0(E-\Sigma)}\right\rangle\ , \tag{4.2}$$

where

$$\mathscr{G}_0(E)=\langle\vec{n}|(E-\hat{\mathscr{H}}_0)^{-1}|\vec{n}\rangle$$

and

$$\hat{\mathscr{H}}_0=-V\sum_{\vec{m},\vec{n}}|\vec{m}\rangle\langle\vec{n}|\ .$$

Obviously

$$V\mathscr{G}_0(E/V)=tG_0(E/t)\ ,$$

where t and G_0 were introduced in Sec. II. The nonlinear Eq. (4.2) was solved numerically for various energies E and disorders W.

In the 1D case there is a complication which deserves special attention. Numerical[11] as well as analytical[12] work has established[2] that the geometric and not the arithmetic average is representative of the ensemble. This strongly suggests that we should calculate the geometric average of $\hat{\mathscr{G}}\equiv(E-\hat{\mathscr{H}})^{-1}$ instead of the arithmetic obtained through Eq. (4.2).

To obtain the geometric average $\langle\hat{\mathscr{G}}(E)\rangle_g$ of $\hat{\mathscr{G}}(E)$ we introduce an effective medium defined by $\Sigma_g(E)$ such that

$$\langle\hat{\mathscr{G}}(E)\rangle_g=\hat{\mathscr{G}}_0(E-\Sigma_g(E))\ . \tag{4.3}$$

To obtain Σ_g we work in a way similar to ordinary CPA; i.e., we replace at an arbitrary site l the effective Σ_g by the actual random site energy ϵ_l, we calculate the resulting Green's function $\hat{\mathscr{G}}'$, and we demand that the average of the *logarithm* of this Green's function equal the logarithm of the average Green's function. The m,n matrix element of $\hat{\mathscr{G}}'(E)$ is given by[2]

$$\mathscr{G}'(m,n;E)=\mathscr{G}_0(m,n;E-\Sigma_g)+\mathscr{G}_0(m,l;E-\Sigma_g)\mathscr{G}_0(l,n;E-\Sigma_g)\times\frac{\epsilon_l-\Sigma_g}{1-(\epsilon_l-\Sigma_g)\mathscr{G}_0(l,l;E-\Sigma_g)}\ . \tag{4.4}$$

The second term in the rhs of Eq. (4.4) becomes significant when l is between m and n. In this case one can show[2] that

$$\mathscr{G}_0(m,l)\mathscr{G}_0(l,n)=\mathscr{G}_0(m,n)\mathscr{G}_0(l,l)\ . \tag{4.5}$$

Substituting Eq. (4.5) into Eq. (4.4) and taking the logarithms of both sides of Eq. (4.4) we obtain

$$\ln\mathscr{G}'(m,n;E)=\ln\mathscr{G}_0(m,n;E-\Sigma_g)-\ln[1-(\epsilon_l-\Sigma_g)\mathscr{G}_0(l,l;E-\Sigma_g)]\ . \tag{4.6}$$

The self-consistency condition that $\langle\ln\mathscr{G}'\rangle=\ln\mathscr{G}_0$ leads to the following nonlinear equation for Σ_g,

$$\langle\ln[1-(\epsilon_l-\Sigma_g)\mathscr{G}_0(l,l;E-\Sigma_g)]\rangle=0\ , \tag{4.7}$$

which replaces the ordinary CPA equation (4.2). It must be pointed out that Eq. (4.7) is valid only in the 1D case because Eq. (4.5) is correct only in the 1D case. One can prove that Σ_g as determined from Eq. (4.7) reproduces through (4.3) exact results for $\langle\mathscr{G}\rangle_g$ in both limits of small and large disorder. It is also worthwhile to mention that Σ_g is different from Σ. In the weak disorder limit

$$\Sigma_g(E)=\tfrac{1}{2}\Sigma(E)=\tfrac{1}{2}\langle\epsilon_l^2\rangle\mathscr{G}_0(E) \tag{4.8}$$

and in the strong disorder limit

$$\Sigma_g(E)\to -iW/2e\ , \tag{4.9}$$

while $\Sigma(E)\to -iW/\pi$ in the same limit.

Having determined the average Green's function one can obtain the mean free path l from the relation[13]

$$\langle\mathscr{G}(\vec{m},\vec{n};E)\rangle=\mathscr{G}_0(\vec{m},\vec{n};E)\exp[-|\vec{m}-\vec{n}|/2l(E)]\ ; \tag{4.10}$$

an average of $l(E)$ over all directions of the vector $\vec{m}-\vec{n}$ is implied in Eq. (4.10). In the weak scattering limit the mean free path $l(E)$ equals $l_2(E)$, where

$$l_2(E)=v(E)\tau(E)\ . \tag{4.11}$$

The relaxation time $\tau(E)=\hbar/2\Sigma_2(E)$, where $\Sigma=\Sigma_1-i\Sigma_2$, and the velocity $v(E)$ equals $v_0(E-\Sigma_1(E))$, where $v_0(E)$ is the magnitude of the velocity for the periodic system described by $\hat{\mathscr{H}}_0$ averaged over the surface of constant energy E. For 2D and 3D systems the equality between l and l_2 is obeyed rather well up to quite large values of the disorder W.

The conductivity σ_0, as given by Eq. (1.1), can be expressed as follows:

$$\sigma_0(E)=\frac{2e^2}{(2\pi)^d d\pi}\int dE' S_0(E-\Sigma_1-E') \times v_0(E-\Sigma_1-E')\frac{\Sigma_2^2}{(E'^2+\Sigma_2^2)^2}\ , \tag{4.12}$$

where $S_0(E)$ is the Fermi surface at E for the periodic system described by $\hat{\mathscr{H}}_0$. We can introduce a length l_1 defined so that

$$\sigma_0(E)=\frac{2}{(2\pi)^d d}\frac{e^2}{\hbar}S(E)l_1(E)\ , \tag{4.13}$$

where $S(E)=S_0(E-\Sigma_1)$. In the weak scattering limit one can easily show[2] that $l_1(E)=l(E)$. However, as the disorder increases, $l_1(E)$ becomes progressively smaller than $l(E)$.

The non-negligible difference between l and l_2 on the one hand and l_1 on the other raises another question: Should one use l or l_1 in Eqs. (3.3)–(3.5)? The basic Eq. (3.1) suggests the use of l_1. On the other hand, since Eq. (3.1) was derived by extrapolating from the weak scattering limit one can equally well argue that l is the appropriate length in Eqs. (3.3)–(3.5). The comparison with existing numerical data cannot settle definitely this issue, although it seems to favor the use of l. In what follows we have used in Eqs. (3.3)–(3.6) the mean free path l as determined by Eq. (4.10) or by Eq. (4.11). We feel that more numerical work is needed especially near the band edges in order to decide which of the various l's fits the data best.

V. RESULTS

A. One-dimensional case

For the one-dimensional case $G_0(E)=(E^2-4t^2)^{-1/2}$. The nearest-neighbor off-diagonal matrix element $g_0(E)$ of $\hat{G}_0$ can in all cases ($d=1,2,3$) be found from the relation

$$EG_0(E)+Ztg_0(E)=1\ . \tag{5.1}$$

In Table I we present our CPA results for the various l's for $E=0$ as the disorder increases from 1 to 20.

To obtain the localization length λ we have used the $\hat{H}_2$ analogy, i.e., Eq. (3.4) with $S=2$, $d=1$, and $l=l_g$. Substituting into Eq. (2.5) we have obtained E_{b2} in terms of l_g, and then, from Eq. (2.7), we have calculated λ. The final result is very simple:

$$\frac{\lambda}{a}=\frac{2}{\ln|1+a/l_g|}\ . \tag{5.2}$$

If $a \ll l_g$ we can expand the logarithm to obtain

$$\lambda \approx 2l_g\ . \tag{5.3}$$

It must be pointed out that the above Eq. (5.3) connecting λ and l_g is exact. The proof is very simple because λ as well as l_g are defined from the decay rate of the geometric average of $\mathscr{G}(n,m)$. The present formalism can produce the exact result $\lambda=2l_g$ only if $a \ll l_g$, which implies that $x_0 \gg 1$, or that the upper cutoff in the integral of Eq.

TABLE I. Various mean free paths (for definition see text) vs disorder W for $E=0$ and $d=1$. Columns 2,3,4 are based on the arithmetic average of $\mathscr{G}$, while columns 5,6,7 are based on the geometric average of $\mathscr{G}$. The unit of length is the lattice spacing.

W/V	l_1	l_2	l	l_{1g}	l_{2g}	l_g
1	23.974	24.173	24.175	48.394	49.172	49.172
2	5.9161	5.9496	5.9556	12.161	12.229	12.232
3	2.5801	2.6299	2.6455	5.4845	5.5181	5.5256
4	1.4175	1.4966	1.5236	3.1408	3.1839	3.1969
5	0.88624	0.99362	1.0329	2.0502	2.1099	2.1293
6	0.60407	0.73188	0.78268	1.4522	1.5299	1.5564
7	0.43739	0.57841	0.63922	1.0868	1.1819	1.2155
8	0.33129	0.47908	0.54830	0.84598	0.95615	0.99676
9	0.25970	0.40987	0.48607	0.67834	0.80066	0.84788
10	0.20925	0.35900	0.44101	0.55650	0.68822	0.74156
11	0.17220	0.31980	0.40669	0.46463	0.60362	0.66257
12	0.14421	0.28866	0.37965	0.39373	0.53788	0.60191
13	0.12255	0.26327	0.35775	0.33789	0.48536	0.55400
14	0.10547	0.24128	0.33964	0.29308	0.44249	0.51527
15	0.091729	0.22432	0.32434	0.25657	0.40683	0.48336
16	0.080531	0.20901	0.31125	0.22647	0.37666	0.45659
17	0.071260	0.19571	0.29987	0.20134	0.35083	0.43382
18	0.063519	0.18406	0.28989	0.18017	0.32841	0.41419
19	0.056978	0.17375	0.28105	0.16212	0.3088	0.39711
20	0.051394	0.16455	0.27314	0.14666	0.29146	0.38208

(1.2) $k_0 \to \infty$.

In Table II we compare the results of the present approach (column labeled $2l_g$) with the numerical data based upon the transmission coefficient (column labeled λ) as well as the results of second-order perturbation theory. The discrepancies between the λ column and the $2l_g$ column are due to errors associated with the CPA-like approach used for the evaluation of the geometric average of the Green's function. In particular the discrepancies for small values of W are due to the breakdown of perturbation theory[14,15] for $E=0$ as $W \to 0$. As a result of this property $\lambda \to 105/W^2$ as $W \to 0$ and not to $96/W^2$ as perturbation theory predicts.[2]

B. Two-dimensional case

The self energy $\Sigma = \Sigma_1 - i\Sigma_2$ is calculated by solving numerically Eq. (4.2), where in the present 2D case[2] $\mathcal{G}_0(E) = 2\mathcal{K}(\lambda)/\pi E$, $\lambda = 4V/E$, and $\mathcal{K}(\lambda)$ is the complete elliptic function of the first kind. To proceed further we need to calculate the product $l(E)S(E) = \tau(E)v(E)S(E) = \tau(E)v_0(E-\Sigma_1)S_0(E-\Sigma_1)$. Since $\tau(E) = \hbar/2\Sigma_2$ is already known we need the product $v_0(E)S_0(E)$ which is equal to

$$v_0(E)S_0(E) = \hbar \,\mathrm{Im} \frac{1}{\pi} \int d\vec{k} \frac{\vec{v}^{\,2}}{E - E(\vec{k})} , \tag{5.4}$$

where $\vec{v} = \vec{\nabla}_{\vec{k}} E(\vec{k})/\hbar$. The integral in Eq. (5.4) can be easily expressed in terms of the Green's functions $\mathcal{G}_0(E)$ and $\mathcal{G}_0(2;E)$, where the latter is the matrix element between the origin and the site (2,0). Thus we have (taking the lattice spacing equal to 1)

$$v_0 S_0 = \frac{4V^2 d(2\pi)^{d-1}}{\hbar} [\,\mathrm{Im}\mathcal{G}_0(E) - \mathrm{Im}\mathcal{G}_0(2;E)] . \tag{5.5}$$

For the 2D square lattice Eq. (5.5) takes the explicit form

$$v_0 S_0 = \frac{32V}{\hbar} \left[\mathcal{E}(k') - \frac{E^2}{(4V)^2} \mathcal{K}(k') \right] , \tag{5.6}$$

where $k'^2 = 1 - E^2/(4V)^2$ and $\mathcal{E}$ is the complete elliptic function of the second kind.

Having thus the product lS we can obtain from Eq. (3.4) the relevant parameter $(Zt/\epsilon')^2$ of the equivalent potential fluctuation. Note that for $d=2$ the spacing a of the equivalent lattice disappears from Eq. (3.4). From $(Zt/\epsilon')^2$ and by employing Eq. (2.5) (which was solved numerically) we obtained E_{b2}; finally, Eq. (2.8) gives the localization length λ. In order to obtain explicit results for λ we need to know a,which is given in terms of l and the constant x_0 [Eqs. (3.7b) and (3.6)]. The quantities l_1, l_2 require for their determination the knowledge of v_0, which can be obtained from the product $v_0 S_0$ [Eq. (5.6)] and S_0. The latter is given by

$$S_0(E) = 8 \int_0^{\varphi_0} d\varphi \left[1 + \frac{\sin^2\varphi}{1 - (|E|/2V - \cos\varphi)^2} \right]^{1/2} , \tag{5.7}$$

TABLE II. Localization length (in units of lattice spacing) vs disorder for $E=0$ and $d=1$. λ is the localization length as determined numerically by the transmission coefficient. The column labeled $2l_g$ presents the results of the present approach and the last column the results of second-order perturbation theory.

W/V	λ	$2l_g$	$\lambda' \equiv 96/W^2$
1	104.3±0.17	98.34	96
2	25.54±0.14	24.46	24
3	11.35±0.02	11.05	10.67
4	6.335±0.01	6.39	6
5	4.088±0.006	4.26	3.84
6	2.935±0.005	3.11	2.67
7	2.285±0.004	2.43	1.96
8	1.883±0.003	1.99	1.5
9	1.612±0.003	1.69	1.19
10	1.415±0.002	1.48	0.96
20	0.76±0.19	0.764	0.24

TABLE III. Various mean free paths (in units of lattice spacing) and the imaginary part of the self-energy vs disorder W for a square lattice at the center of the band ($E=0$).

W/V	l_1	l_2	l	Σ_2/V
2	3.86	3.94	4.0	0.229
3	1.97	2.03	2.04	0.445
4	1.23	1.28	1.30	0.703
5	0.844	0.911	0.917	0.991
6	0.619	0.694	0.689	1.30
7	0.475	0.556	0.556	1.62
8	0.376	0.461	0.466	1.96
9	0.305	0.393	0.407	2.29
10	0.252	0.342	0.355	2.64
11	0.211	0.303	0.320	2.98
12	0.180	0.272	0.295	3.32
13	0.154	0.247	0.267	3.66
14	0.135	0.226	0.249	4.00
15	0.118	0.210	0.234	4.35

TABLE IV. Comparison of our results [λ (present)] for the localization length λ in a disordered square lattice at $E=0$ with the numerical data of Refs. 16 and 17 [λ (MK)] for various values of the disorder W. The unit of length is the lattice spacing.

W/V	λ (present)	λ (MK)[a]	λ (MK)[b]
2	6.34×10^8		7.994×10^6
3	47 234		5046
4	1123		481
5	147	110	97.58
6	41.26	37.6	37.46
7	18.79	18.24	18.53
8	10.91	10.64	11.07
9	7.54	6.81	7.296
10	5.34	5.12	5.451
12	3.50	3.20	3.443
15	2.17	2.03	2.200

[a]From MacKinnon and Kramer, Ref. 16.
[b]From MacKinnon and Kramer, Ref. 17.

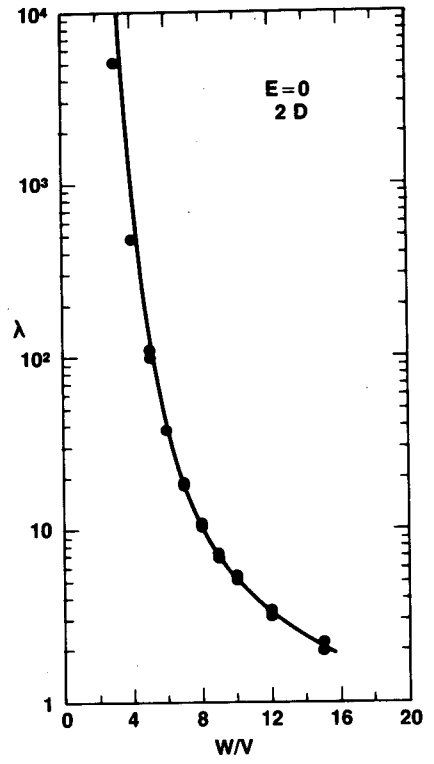

FIG. 1. Localization length λ (in units of lattice spacing) vs disorder W for a square lattice at the center of the band ($E=0$). Solid line represents the results of the present work and the points are the numerical data of Refs. 16 and 17.

where $\cos\varphi_0 = |E|/4V$. For $E=0$, $S_0 = 4\sqrt{2}\pi$, $v_0 = 4\sqrt{2}V/\pi\hbar$, and

$$l_2 = \frac{2\sqrt{2}}{\pi}\frac{V}{\Sigma_2} \tag{5.8}$$

in units of lattice spacing. In Table III we present results for l_1 [Eq. (4.13)], l_2 [Eq. (5.8)], and l [Eq. (4.10)].

Our results for λ are in reasonable agreement with the numerical data of MacKinnon and Kramer[16,17] for the center of the band if one chooses x_0 to be 1.14. This is shown in Table IV and Fig. 1. Our results seem to be larger than the estimates of Refs. 16 and 17 for weak disorder. However, in the weak disorder limit the method of Refs. 16 and 17 becomes less accurate. Thus it is not presently clear whether or not the potential-well analogy presented here overestimates λ for weak disorder. Anyway, for weak disorder our result for λ has the following simple analytical form (choosing $x_0 = 1.14$) for the center of the band:

$$\lambda \approx 2.72 l e^{\sqrt{2}\pi l}, \tag{5.9}$$

where all lengths are given in units of lattice spacing. It is worthwhile to point out that Eq. (5.9) works reasonably well for W/V up to 8 and that for weak disorder λ grows extremely fast, e.g., for $W=2$, $\lambda \sim 10^8 \sim 1$ cm, i.e., it becomes of macroscopic scale.

C. Three-dimensional case

As in the 2D case the self-energy $\Sigma = \Sigma_1 - i\Sigma_2$ is calculated by solving numerically Eq. (4.2). In the present case

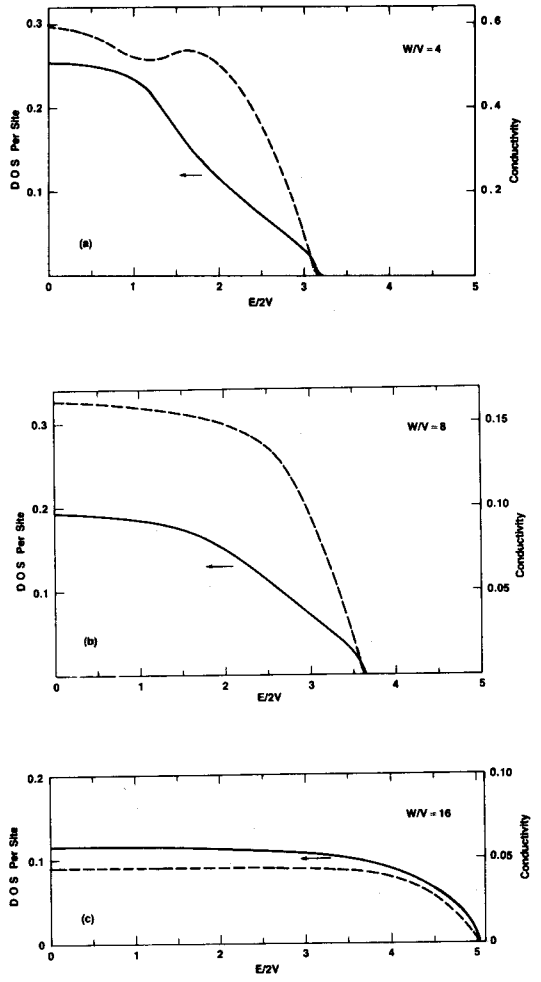

FIG. 2. Density of states per site [solid line in units of $(2V)^{-1}$] and classical conductivity σ_0 (dashed line in units of $e^2/\hbar a_0$, where a_0 is the lattice spacing) vs $E/2V$ for three different values of the disorder in a cubic lattice.

$\mathcal{G}_0(E)$ is given as an integral of elliptic functions (see, e.g., Ref. 2).

To obtain the conductivity one needs the product $v_0 S_0$ which is given by Eq. (5.5). The function $\mathcal{G}_0(2;E)$ is tabulated in Ref. 2. In Fig. 2 we plot the DOS per site and the conductivity σ_0 versus E for various values of the disorder. It is worthwhile to point out that the rather strong structure which appears in σ_0 for $E/V \approx \pm 2$ and $W=4V$ is a remnant of the Van Hove singularities at $E/V = \pm 2$.

To obtain $S_0(E)$, and hence $v_0(E)$, we use the integral

$$S_0(E) = 8\int_0^{\varphi_{10}} d\varphi_1 \int_0^{\varphi_{20}} d\varphi_2 \frac{1}{\cos\theta}, \tag{5.10}$$

where

$$\cos\varphi_{10} = \frac{E}{2V} - 2 \text{ if } \left|\frac{E}{2V} - 2\right| \le 1, \tag{5.11}$$

and

$$\varphi_{10}=\pi \text{ if } \left|\frac{E}{2V}-2\right|>1 ,$$

$$\cos\varphi_{20}=(|E|/2V)-1-\cos\varphi_1 \quad \text{if } |(|E|/2V)-1-\cos\varphi_1|\le 1 ,$$

$$\varphi_{20}=\pi \text{ if } |(|E|/2V)-1-\cos\varphi_1|>1 , \tag{5.12}$$

$$\frac{1}{\cos\theta}=(\sin^2\varphi_1+\sin^2\varphi_2+1-\cos^2\varphi_3)^{1/2}/(1-\cos^2\varphi_3)^{1/2} , \tag{5.13}$$

$$\cos\varphi_3=(|E|/2V)-\cos\varphi_1-\cos\varphi_2 \quad \text{if } |(|E|/2V)-\cos\varphi_1-\cos\varphi_2|\le 1 ,$$

$$\varphi_{30}=(1+\sin^2\varphi_1+\sin^2\varphi_2)^{1/2} \quad \text{if } |(|E|/2V)-\cos\varphi_1-\cos\varphi_2|>1 . \tag{5.14}$$

Near the ends of the band $S(E)$ can be approximated by

$$S_0(E)\approx 4\pi\left[6-\frac{|E|}{V}\right] . \tag{5.15}$$

In Figs. 3 and 4 we plot $S(E)=S_0(E-\Sigma_1)$ and the mean free paths $l_1(E)$ and $l_2(E)\approx l$ versus E for various values of the disorder.

To find the mobility edge one can utilize either the $\hat{H}_1$ [Eq. (3.3)] or the $\hat{H}_2$ [Eq. (3.5)] analogy, since both predict by design the same critical disorder. For simplicity we utilize the $\hat{H}_1$ analogy.

The critical value for the appearance of a bound state in a single potential well is

$$\frac{Zt}{|\epsilon|}=ZtG_0(Zt)=1.516\,386 , \tag{5.16}$$

where the last equality follows from Table 5.2 of Ref. 2. Combining Eq. (5.16) with Eq. (3.3) we obtain the following equation for the position of the mobility edge:

$$l^2S=12x_0 . \tag{5.17}$$

Equation (5.17) is very significant. At the center of the band where S is proportional to square of the inverse of the lattice spacing, Eq. (5.17) implies immediately that the states become localized when the mean free path becomes comparable to the interatomic distance. This is the localization criterion championed by Mott.[18] However, near the band edge for weak disorder S is much smaller than its value at the center of the band. Hence Eq. (5.17) implies that the mean free path at the mobility edge near the band edge could be much larger than the interatomic separation. This implication is in clear disagreement with the prevailing belief that in order to reach localization one has first to reduce the mean free path (i.e., the phase coherence length) to interatomic distances. According to Eq. (5.17) for weak disorder near the band edge (which is actually the most common case for a lot of materials) the amplitude of the eigenfunctions becomes inhomogeneous and eventually decays to zero for large distance *before* the phase coherence length has a chance to become comparable to interatomic distances.

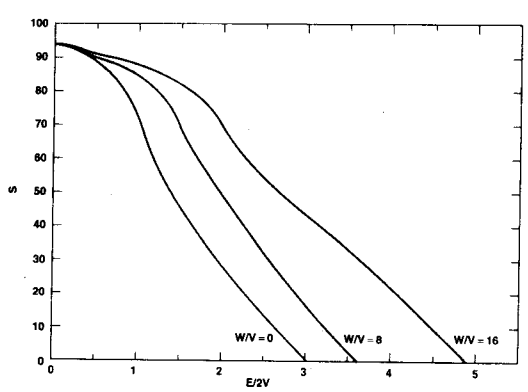

FIG. 3. Fermi surface $S(E)=S_0(E-\Sigma_1)$ vs $E/2V$ for three different values of the disorder W for a cubic lattice. The unit of length is the lattice constant.

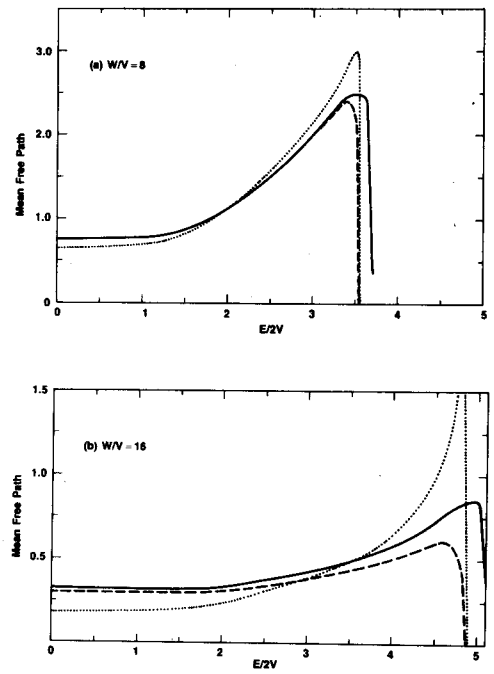

FIG. 4. Mean free paths l (solid line), l_2 (dashed line), and l_1 (dotted line) vs $E/2V$ for two different values of the disorder W for a cubic lattice. The unit of length is the lattice constant.

In order to check the predictions of Eq. (5.17) one needs independent numerical data for the position of the mobility edge. Such data exist[1] for the center of the band ($E=0$). In order to fit the critical value $W_c/V\approx 16.5$ estimated in Ref. 17 one must choose x_0 in Eq. (5.17) as follows:

$$x_0=0.745\approx 0.75 . \tag{5.18}$$

Of course the most interesting region to check is near the band edge for weak disorder. This is not only the most relevant case but it is there that the present approach predicts a behavior qualitatively different from the generally accepted one. Unfortunately, to the best of our knowledge, there are no independent numerical data in this regime. Until such data (probably based on the tech-

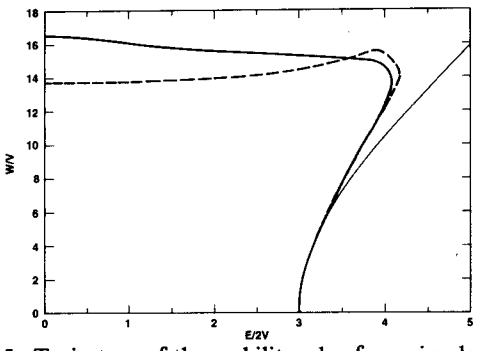

FIG. 5. Trajectory of the mobility edge for a simple cubic lattice as predicted by the present work (solid line) and by the $L(E)$ method (dashed line). The CPA band edges are also indicated (thin solid line).

nique of Refs. 19 or 20) appear it is not possible to decide whether the behavior at the mobility edge near the band edge is as implied by Eq. (5.17) or as described in Ref. 18.

In Fig. 5 we present our predictions [based on Eqs. (5.17) and (5.18)] for the trajectory of the mobility edge. In the same figure the corresponding results based upon the $L(E)$ method[21] are shown together with the CPA band edges.

It is worthwhile to point out that at the center of the band and at the critical disorder W_c ($W_c/V \approx 16.5$) the mean free path l_c is considerably smaller than the interatomic distance ($l_c = 0.3079 \approx \frac{1}{3}$). The localization length for $W > W_c$ can be found by combining Eqs. (2.5), (2.8), and (3.5) or Eqs. (2.4), (2.8), and (3.3). For W close to W_c (actually up to $W/V \approx 30$) $2tG_0(E) \approx 0.505\,462 - b(|E|/t-6)^{1/2} = 0.505\,462 - ba/\lambda$ with $b = 0.1666$. We then have

$$\lambda = Ca/S(a_c l_c - al) . \tag{5.19}$$

In view of Eqs. (3.6) and (3.7c) (which imply that $a \sim l/x_0$), the proportionality constant x_0 drops out of Eq. (5.19) which becomes

$$\lambda = Cl/S(l_c^2 - l^2) . \tag{5.20}$$

On first sight, one may be tempted to interpret the dropping out of x_0 as meaning that λ is independent of the length scale of the effective medium. Actually this is not the case, because the quantity C turns out to be model dependent and to increase with the number of sites involved in the potential well ($C \approx 19.72$ for the $\hat{H}_1$ analogy and $C = 29.44$ for the $\hat{H}_2$ analogy). This feature, on the one hand, restores the expected increase of λ with the size of the potential well (or fluctuation); on the other hand, it creates an uncertainty regarding the proper value of C. One may argue on physical grounds that C must decrease with increasing disorder approaching in the limit $W \to \infty$ the value corresponding to a single potential well, $C_\infty = 19.72$; furthermore, the dimensionless quantity C must be a function of the only relevant dimensionless quantity in the problem: Sl.[2] The simple choice $C = ASl^2 + C_\infty$ leads to the following equation for λ:

$$\lambda = \frac{(0.213 + Al^2)l}{l_c^2 - l^2} \tag{5.21}$$

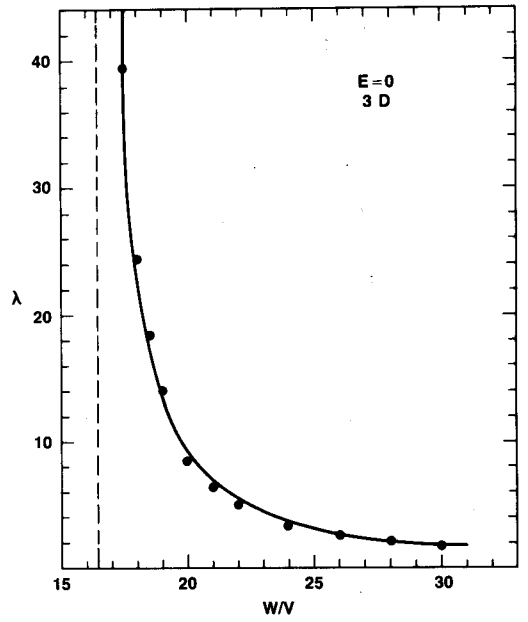

FIG. 6. Localization length λ (in units of lattice constant) vs disorder W for a 3D simple cubic model at the center of the band ($E=0$). Solid line represents the results of the present work and the points are numerical data of Ref. 17. The critical disorder below which all states are extended is taken as $W_c \cong 16.5V$.

which for $A = 12.5$ produces results in fair agreement with the numerical data of Ref. 17 as shown in Fig. 6.

VI. CONCLUSIONS

We have shown in the present work that the results produced by the equivalent local potential fluctuation are consistent with the existing independent numerical data on the problem of the localization length. They are also in fair agreement with the results based on the $L(E)$ method.[21]

The dimensionless local potential well (or fluctuation) of the equivalent problem is proportional to the dimensionless product Sla^{d-2}, where S is the Fermi surface, l is the mean free path, and a is a length scale in the equivalent problem (corresponding to an upper cutoff in momentum integrals). In order to obtain explicit results one must make certain choices: (a) about the appropriate definition of S in a disordered system; (b) about whether (or not) one must use l_1 in the place of l; and (c) about the connection of a with l (or l_1), S, and the interatomic spacing. In the present work, on the basis of a better agreement with numerical data we have made the following choices: (a) we took $a \sim l$, (b) we used the mean free path l as defined by the decay of the off-diagonal matrix elements of the average Green's function, and (c) we took $S(E) = S_0(E - \Sigma_1)$. We have also examined as a definition of $S(E)$ the reasonable choice of averaging $S_0(E - \Sigma_1)$ over a region of width Σ_2. Then (If one still employs the choice $a \sim l$) the main difference is that the trajectory of the mobility edge has a shape like that of the $L(E)$ method with a more pronounced maximum at $E \approx 5$

reaching $W \approx 20$. One has no reasons to expect such a behavior of the mobility edge trajectory.

The numerical data are not numerous enough and/or so accurate as to exclude choices other than the ones made in the present study. We have obtained simple formulas expressing the localization length in terms of the mean free path [see Eqs. (5.3), (5.9), and (5.21)].

The most important new result of the present work is Eq. (5.17) which says that the mobility edge is reached when the product $l^2 S = \text{const}$. At the center of the band this condition reduces to Mott's criterion stating that localization is taking place when l is comparable to (actually about $\frac{1}{3}$ of) the interatomic distance. However, for the important and very common case of weak disorder and energy near the band edge our criterion (5.17) predicts that localization can take place while the mean free path is still much larger than the interatomic distance. Further numerical work near the band edge for weak disorder is needed in order to check the correctness of this important prediction.

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†Present address: Department of Physics, Iowa State University, Ames, IA 50011.

*Permanent address: Department of Physics, University of Crete and Research Center of Crete, Heraklio, Crete, Greece.

[1]E. N. Economou and C. M. Soukoulis, Phys. Rev. B **28**, 1093 (1983).

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

[3]L. P. Gor'kov, D. Khmelnitzkii, and A. I. Larkin, Pis'ma Zh. Eksp. Teor. Fiz. **30**, 248 (1979) [JETP Lett. **30**, 228 (1979)].

[4]D. Vollhardt and P. Wölfle, Phys. Rev. Lett. **48**, 699 (1982); Phys. Rev. B **22**, 4666 (1980).

[5]M. H. Cohen and E. N. Economou (unpublished).

[6]F. J. Wegner, Z. Phys. B **25**, 327 (1976); **35**, 207 (1979).

[7]E. A. Kotov and M. V. Sadovskii, Z. Phys. B **51**, 17 (1983).

[8]M. Kaveh and N. F. Mott, J. Phys. C **14**, L177 (1981); **14**, L659 (1981).

[9]A. V. Myasnikov and M. V. Sadovskii, Fiz. Tverd. Tela (Leningrad) **24**, 3569 (1982).

[10]D. W. Taylor, Phys. Rev. **156**, 1017 (1967); P. Soven, *ibid.* **156**, 809 (1967).

[11]E. N. Economou and C. M. Soukoulis, Phys. Rev. Lett. **46**, 618 (1981); B. S. Andereck and E. Abrahams, J. Phys. C **13**, L383 (1980); J. Sak and B. Kramer, Phys. Rev. B **24**, 1761 (1981).

[12]A. A. Abrikosov, Solid State Commun. **37**, 997 (1981).

[13]A. A. Abrikosov, L. P. Gor'kov, and I. E. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Englewood Cliffs, N. J., 1963).

[14]M. Kappus and F. Wegner, Z. Phys. B **45**, 15 (1981).

[15]S. Sarker, Phys. Rev. B **25**, 4304 (1982).

[16]A. MacKinnon and B. Kramer, Phys. Rev. Lett. **49**, 695 (1982).

[17]A. MacKinnon and B. Kramer, Z. Phys. B **53**, 1 (1983).

[18]See, e.g., N. F. Mott and E. A. Davis, *Electronic Processes in Non-Crystalline Materials*, 2nd ed. (Clarendon, Oxford, 1979).

[19]A. MacKinnon and B. Kramer, Phys. Rev. Lett. **47**, 1546 (1981).

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

[21]D. C. Licciardello and E. N. Economou, Phys. Rev. B **11**, 3697 (1975). In Fig. 5 we have employed a slightly improved localization function, which, however, produces results essentially identical to those obtained by Licciardello and Economou. The improved localization function is $L(E)=KV|t|^{1/3}$, where $K=4.6826$, $t=D/\mathcal{G}_0$, and $D=\{[\mathcal{G}_0+\mathcal{G}_0(1,1,0)]^2-4\mathcal{G}_0^2(1,0,0)\}[\mathcal{G}_0-\mathcal{G}_0(1,1,0)]^2$. The argument of all Green's function is $E-\Sigma(E)$. Taking into account that $|\mathcal{G}_0(1,1,0)| \ll |\mathcal{G}_0(1,0,0)| \ll |\mathcal{G}_0|$ we can approximate the above $L(E)$ as follows $L(E) \approx KV|\mathcal{G}_0-4\mathcal{G}_0^2/3\mathcal{G}_0(1,0,0)|$.