

Effect of correlations on the localization properties of electrons and phonons in the long-wavelength limit

Qian-Jin Chu

Institute of Physics, Chinese Academy of Sciences, Beijing, China

Zhao-Qing Zhang

*Center of Theoretical Physics, CCAST (World Laboratory) P.O. Box 8730, Beijing, China
and Institute of Physics, Chinese Academy of Sciences, Beijing, China*

(Received 11 October 1988)

The problem of Anderson localization in a spatially correlated disordered potential is formulated in the framework of the self-consistent theory of Vollhardt and Wolfe in conjunction with the self-consistent Born approximation for both tight-binding electrons and phonons. An approximation which is exact in the weak scattering limit is introduced for the coherent backscattering contribution to the irreducible two-particle vertex. For the case of electrons in three dimensions, the phase diagrams in the near-band-edge region are studied numerically for the binary alloys with short-range correlations and the idea of quasiuniversality is examined. For the case of phonons in one and two dimensions, the complete expressions for the localization length are obtained in the long-wavelength limit for both short-range and long-range correlations. The universality holds when the correlations are short range. In the presence of long-range correlations, different expressions for the localization length are obtained depending on the definition of the mean free path used in the theory. When the single-phonon mean free path is used, our results give the same asymptotic behaviors found previously by using the replica method. In one dimension, different asymptotic behavior appears when the transport mean free path is used. Discussions are given.

I. INTRODUCTION

In the past decade, considerable progress has been made in understanding the localization properties of independent electrons in a random potential.¹ Anderson localization, as a result of the multiple scattering of waves due to the random potential, is recognized to be common to electrons, phonons, and various kinds of classical waves.²⁻⁴ It is now generally believed that in dimension $d \leq 2$ all the states are localized. For the tight-binding electrons in $d = 3$, the phase diagrams of the Anderson transition have been studied numerically using the finite-size scaling method for various types of random potential.^{5,6} By taking into account the coherent backscattering effect, the self-consistent diagrammatical theory developed by Vollhardt and Wolfe⁷ (VW) in conjunction with the coherent-potential approximation (CPA) has been shown to be very successful in determining the localization phase diagram.^{5,8} This diagrammatical theory has also been used to study the localization properties of the electromagnetic waves,⁹ scalar waves,^{10,11} and phonons,^{12,13} etc.

For most of the studies in the past, the disordered potentials are assumed to be completely random at different lattice sites in the discrete models and a finite correlation length is always assumed in the continuous models. Recently, attention has been focused on the effects of the correlations among the disordered potential to the localization and transport properties of the system. For the case of scalar waves, it has been shown by using the replica-field-theory method that the correlations are im-

portant to the localization properties.¹⁴ In particular, for the case of long-range correlations with a power-law decay of the form $(a^2 + r^2)^{-n}$, the long-wavelength asymptotic behaviors for the localization length in $d = 1$ and 2 are found to be n dependent. For the case of tight-binding electrons, the effects of the short-range correlations to the localization properties have been studied by various methods in $d = 1$.^{15,16} In $d = 3$, the effects of the short-range correlations to the conductivity have been studied for the binary alloys in the metallic limit by including the correlations in both the bare conductivity and the coherent backscattering correction.¹⁷ Independently, we have generalized the theory of VW in the context of self-consistent Born approximation (SCBA) to include the correlations in the disordered potential.¹⁸ For an exponential decay correlation, the phase diagram in the near-band-edge region is found to be strongly correlation dependent.

In this work we will briefly derive the generalization of the theory of VW in the context of SCBA to include the correlations in the disordered potential for both tight-binding electrons and phonons. An approximation which is exact in the weak scattering limit is introduced for the coherent backscattering contribution to the irreducible two-particle vertex. For the case of electrons in $d = 3$, we have investigated the phase diagram numerically in the near-band-edge region for the binary alloys with short-range correlations. This is the region where SCBA is valid. Even outside this region, the SCBA is believed to give a phase diagram which is qualitatively correct.¹⁹ The idea of quasiuniversality predicted by reduction to the

white-noise model (WNM) in the long-wavelength limit will be examined.²⁰ For the case of phonons in $d = 1$ and 2, up to an arbitrary constant of order unity, the complete expressions for the localization length and other physical quantities are obtained in the long-wavelength limit for both short-range and long-range correlations. In the case of short-range correlations, all the physical quantities follow universal behaviors as predicted by the reduction to the WNM. In the case of long-range correlations, different expressions are obtained depending on the definition of the mean free path used in the theory. When the single-phonon mean free path is used, our results give the same asymptotic behaviors found previously by using the replica method.¹⁴ In $d = 1$, except for one particular case, different asymptotic behavior appears when the transport mean free path is used. In $d = 2$, different prefactors may appear. The use of a transport mean free path also introduces another length scale to the problem and raises the question of the validity of the single-parameter scaling theory in the presence of long-range correlations.

In Sec. II the theory of VW is formulated in the presence of correlations for the tight-binding electrons. In Sec. III the phase diagrams for the three-dimensional binary alloys with short-range correlations are investigated in the near-band-edge region and the quasiuniversality is discussed. The formulations for the case of phonons are given in Sec. IV. In Sec. V the complete expressions for the localization length are given for $d = 1$ and 2 in the long-wavelength limit for both short-range and long-range correlations. Conclusions and discussions are given in Sec. VI.

II. FORMULATIONS FOR THE CASE OF TIGHT-BINDING ELECTRONS

Considering a single-band tight-binding Hamiltonian for independent electrons in a d -dimensional lattice with the lattice constant a ,

$$H = \sum_i \varepsilon_i |i\rangle \langle i| + t \sum_{\langle i,j \rangle} |i\rangle \langle j|, \quad (1)$$

where t is the constant nearest-neighbor hopping matrix and ε_i is the site energy at site i with the probability distribution $P(\varepsilon_i)$. In the presence of correlations, the two-site correlation function for the site energies ε_i and ε_j can be denoted as $\langle \varepsilon_i \varepsilon_j \rangle = W^2 C(\mathbf{R}_i - \mathbf{R}_j)$ where W^2 is the variance of the distribution function $P(\varepsilon_i)$ and the correlation function C is normalized by $C(0) = 1$. In the SCBA, the averaged single-particle Green's function $\langle G(z) \rangle [= R(z), z = E \pm i\eta]$ is determined by the following equations, in the momentum representation:¹⁸

$$R_p^\pm(E) = \langle \mathbf{p} | R(E \pm i\eta) | \mathbf{p} \rangle = [E - \varepsilon(\mathbf{p}) - \Sigma_p^\pm(E)]^{-1}, \quad (2)$$

$$\Sigma_p^\pm(E) = \frac{W^2}{N} \sum_{\mathbf{p}'} S(\mathbf{p} - \mathbf{p}') R_{\mathbf{p}'}^\pm(E), \quad (3)$$

$$S(\mathbf{q}) = \sum_i C(\mathbf{R}_i) e^{i\mathbf{q} \cdot \mathbf{R}_i}, \quad (4)$$

and

$$\varepsilon(\mathbf{p}) = t \sum_{\delta} e^{i\mathbf{p} \cdot \delta}, \quad (5)$$

where the superscripts “+” and “-” stand for the retarded and advanced Green's functions and δ represents all the nearest-neighbor vectors. $S(\mathbf{q})$ is the structure function which is identical to one in the absence of the correlations, i.e., $C(\mathbf{R}_i - \mathbf{R}_j) = \delta_{ij}$.

To study the transport and localization properties, we follow the main steps of VW (Ref. 7). The Bethe-Salpeter equation for the averaged two-particle Green's function $\phi_{\mathbf{p},\mathbf{p}'}^E(\mathbf{q}, \omega)$ has the following form for small q :

$$\phi_{\mathbf{p},\mathbf{p}'}^E(\mathbf{q}, \omega) = \frac{-1}{2\pi i} \langle G_{\mathbf{p}+\mathbf{p}'}^+(E_+) G_{\mathbf{p}'-\mathbf{p}}^-(E_-) \rangle, \quad (6)$$

$$\begin{aligned} & [\omega - \mathbf{q} \cdot \mathbf{V}_p - \Sigma_{\mathbf{p}+}^+(E_+) + \Sigma_{\mathbf{p}-}^-(E_-)] \phi_{\mathbf{p},\mathbf{p}'}^E(\mathbf{q}, \omega) \\ &= \Delta R_p^E(\mathbf{q}, \omega) \left[\frac{\delta_{\mathbf{p},\mathbf{p}'}}{2\pi i} - \sum_{\mathbf{p}''} U_{\mathbf{p},\mathbf{p}''}^E(\mathbf{q}, \omega) \phi_{\mathbf{p}'',\mathbf{p}}^E(\mathbf{q}, \omega) \right], \quad (7) \end{aligned}$$

with

$$\mathbf{p}_\pm = \mathbf{p} \pm \frac{\mathbf{q}}{2}, \quad E_\pm = E \pm \frac{\omega}{2}, \quad (8)$$

and

$$\mathbf{V}_p = \frac{\partial \varepsilon(\mathbf{p})}{\partial \mathbf{p}}, \quad \Delta R_p^E(\mathbf{q}, \omega) = R_{\mathbf{p}+}^+(E_+) - R_{\mathbf{p}-}^-(E_-). \quad (9)$$

The function $U_{\mathbf{p},\mathbf{p}'}^E(\mathbf{q}, \omega)$ is the two-particle vertex in the particle-hole channel. Two classes of important diagrams for U are shown in Fig. 1. Figure 1(a) shows the Born approximation vertex while Fig. 1(b) shows the maximally crossed diagrams which are responsible for the localization effect. Here, every interaction line in U associates with a structure function S (or a correlation function C in the real-space representation). Summing both sides of Eq. (7) over \mathbf{p} and \mathbf{p}' and using the Ward identity, the following equation is obtained in the small q and ω limit:

$$\omega \phi^E(\mathbf{q}, \omega) - q \phi_j^E(\mathbf{q}, \omega) = -N \rho(E), \quad (10)$$

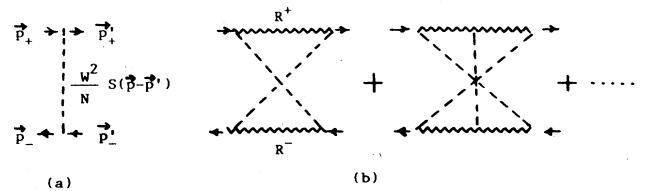


FIG. 1. Two important classes of diagrams for the two-particle vertex U in the momentum representation, (a) for the Born approximation, (b) for the maximally crossed diagrams. R^+ and R^- are, respectively, the averaged single-particle retarded and advanced Green's functions. Every interaction line (dotted lines) is now associated with a structure function S . W^2 is the variance of the site energy distribution.

with

$$\phi^E(\mathbf{q}, \omega) = \sum_{\mathbf{p}, \mathbf{p}'} \phi_{\mathbf{p}, \mathbf{p}'}^E(\mathbf{q}, \omega),$$

$$\phi_j^E(\mathbf{q}, \omega) = \sum_{\mathbf{p}, \mathbf{p}'} (\mathbf{V}_{\mathbf{p}} \cdot \hat{\mathbf{q}}) \phi_{\mathbf{p}, \mathbf{p}'}^E(\mathbf{q}, \omega),$$

and

$$\rho(E) = \frac{-1}{2\pi i N} \sum_{\mathbf{p}} \Delta R_{\mathbf{p}}(E), \quad (11)$$

where $\Delta R_{\mathbf{p}}(E)$ is equal to $\Delta R_{\mathbf{p}}^E(0, 0)$ of Eq. (9) and $\rho(E)$ is the electron density of state per site. To obtain the current relaxation equation for $\phi_j^E(\mathbf{q}, \omega)$ we multiply Eq. (7) by $(\mathbf{V}_{\mathbf{p}} \cdot \hat{\mathbf{q}})$ and sum over \mathbf{p} and \mathbf{p}' again. With the use of the expansion^{7,19}

$$\begin{aligned} \phi_{\mathbf{p}}^E(\mathbf{q}, \omega) &= \sum_{\mathbf{p}'} \phi_{\mathbf{p}, \mathbf{p}'}^E(\mathbf{q}, \omega) \\ &\cong \frac{-1}{2\pi i \rho(E) N} \Delta R_{\mathbf{p}}(E) \\ &\quad \times \sum_{\mathbf{p}', \mathbf{p}''} \left[1 + \frac{(\mathbf{V}_{\mathbf{p}} \cdot \hat{\mathbf{q}})(\mathbf{V}_{\mathbf{p}''} \cdot \hat{\mathbf{q}}) d}{V_E^2} \right] \phi_{\mathbf{p}', \mathbf{p}''}^E(\mathbf{q}, \omega), \end{aligned} \quad (12)$$

with the mean group velocity V_E defined as

$$V_E^2/d = \frac{-1}{2\pi i \rho(E) N} \sum_{\mathbf{p}} (\mathbf{V}_{\mathbf{p}} \cdot \hat{\mathbf{q}})^2 \Delta R_{\mathbf{p}}(E), \quad (13)$$

the equation for $\phi_j^E(\mathbf{q}, \omega)$, after some manipulations, becomes

$$[\omega + M^E(\mathbf{q}, \omega)] \phi_j^E(\mathbf{q}, \omega) - \frac{q^2 V_E^2}{d} \phi^E(\mathbf{q}, \omega) = 0, \quad (14)$$

with

$$\begin{aligned} M^E(\mathbf{q}, \omega) &= \frac{d}{2\pi i \rho(E) V_E^2 N} \left[\sum_{\mathbf{p}} (\mathbf{V}_{\mathbf{p}} \cdot \hat{\mathbf{q}})^2 \Delta R_{\mathbf{p}}(E) [\Sigma_{\mathbf{p}_+}^+(E_+) - \Sigma_{\mathbf{p}_-}^-(E_-)] \right. \\ &\quad \left. - \sum_{\mathbf{p}, \mathbf{p}'} (\mathbf{V}_{\mathbf{p}} \cdot \hat{\mathbf{q}}) \Delta R_{\mathbf{p}}(E) U_{\mathbf{p}, \mathbf{p}'}^E(\mathbf{q}, \omega) \Delta R_{\mathbf{p}'}(E) (\mathbf{V}_{\mathbf{p}'} \cdot \hat{\mathbf{q}}) \right]. \end{aligned} \quad (15)$$

Solving Eqs. (10) and (14), to the leading order in q and ω , we find

$$\phi^E(\mathbf{q}, \omega) = \frac{i\rho(E)N}{-i\omega + D(\omega, E)q^2}, \quad (16)$$

$$\phi_j^E(\mathbf{q}, \omega) = \frac{qD(\omega, E)\rho(E)N}{-i\omega + D(\omega, E)q^2}, \quad (17)$$

with

$$D(\omega, E) = \frac{iV_E^2}{dM^E(0, \omega)}. \quad (18)$$

In the region of extended states, $D(0^+, E)$, denoted as $D(E)$, is the diffusion constant which is related to the dc conductivity $\sigma(E)$ by the Einstein relation $\sigma(E) = 2e^2 \rho(E) D(E) / \hbar a^d$. With the use of Eq. (3) and the Born approximation (BA) for U [Fig. 1(a)],

$$U_{\mathbf{p}, \mathbf{p}'}^{(\text{BA})}(\mathbf{q}, \omega) = \frac{W^2}{N} S(\mathbf{p} - \mathbf{p}'), \quad (19)$$

in Eq. (15), we find that the bare diffusion constant $D_{\text{BA}}(E)$ of Eq. (18) becomes

$$\begin{aligned} D_{\text{BA}}(E) &= \frac{iV_E^2}{dM^{(\text{BA})}(0, 0^+)} \\ &= \frac{-2\pi\rho(E)V_E^4}{\frac{d^2 W^2}{N^2} \sum_{\mathbf{p}, \mathbf{p}'} \Delta R_{\mathbf{p}}(E) S(\mathbf{p} - \mathbf{p}') \Delta R_{\mathbf{p}'}(E) (\mathbf{V}_{\mathbf{p}} \cdot \hat{\mathbf{q}}) (\mathbf{V}_{\mathbf{p}'} \cdot \hat{\mathbf{q}})}. \end{aligned} \quad (20)$$

The contribution of the maximally crossed diagrams to U [Fig. 1(b)] can be summed using the time reversal symmetry, yielding

$$\delta U_{\mathbf{p}, \mathbf{p}'}^{(M)}(0, \omega) = \frac{W^4}{N^2} \sum_{\mathbf{p}_1, \mathbf{p}_2} S(\mathbf{p}_1 + -\mathbf{p}) S(\mathbf{p}' - \mathbf{p}_2) \phi_{\mathbf{p}_1, \mathbf{p}_2}^{(\text{BA})}(\mathbf{q}, \omega), \quad (21)$$

where $\mathbf{q} = \mathbf{p} + \mathbf{p}'$ and $\phi_{\mathbf{p}_1, \mathbf{p}_2}^{(\text{BA})}(\mathbf{q}, \omega)$ is the Born approximation to the function $\phi_{\mathbf{p}_1, \mathbf{p}_2}^E(\mathbf{q}, \omega)$ of Eq. (6) or (7). In order to evaluate Eq. (21), we introduce an approximation by taking into account the fact that the function $\phi_{\mathbf{p}_1, \mathbf{p}_2}^{(\text{BA})}(\mathbf{q}, \omega)$ has the peaked values when $\mathbf{p}_1 = \mathbf{p}_2$ as can be seen from Eq. (7). This is particularly true when $U^{(\text{BA})}$ of Eq. (19) is small. Thus Eq. (21) can be approximated by

$$\begin{aligned} \delta U_{\mathbf{p},\mathbf{p}'}^{(M)}(0,\omega) &\cong \frac{W^4}{N^2} \sum_{\mathbf{p}_1} S(\mathbf{p}_{1+}-\mathbf{p})S(\mathbf{p}'-\mathbf{p}_{1+}) \sum_{\mathbf{p}_2} \phi_{\mathbf{p}_1,\mathbf{p}_2}^{(BA)}(\mathbf{q},\omega) \\ &= \frac{W^4}{N^2} \sum_{\mathbf{p}_1} S(\mathbf{p}_{1+}-\mathbf{p})S(\mathbf{p}'-\mathbf{p}_{1+}) \frac{i\Delta R_{\mathbf{p}_1}(E)}{-i\omega + D_{BA}(E)|\mathbf{p}+\mathbf{p}'|^2}, \end{aligned} \quad (22)$$

where the Born approximation solutions $\phi^{(BA)}(\mathbf{q},\omega)$ and $\phi_j^{(BA)}(\mathbf{q},\omega)$ of Eqs. (16) and (17) have been used in Eq. (12) to obtain the last equation of Eq. (22). With the use of $M^{(BA)}$ in Eq. (20) and the result of $\delta U^{(M)}$ in Eq. (15), the self-consistent equation for the renormalized diffusion constant $D(\omega,E)$ can be obtained following the procedure of VW, yielding

$$D(\omega,E) = D_{BA}(E) \left[1 - \frac{\beta(E)}{N} \sum_{\mathbf{q}}' \frac{1}{q^2 - i\omega/D(\omega,E)} \right], \quad (23)$$

with

$$\begin{aligned} \beta(E) &= \frac{dW^4}{2\pi i \rho(E) V_E^4 N^2} \sum_{\mathbf{p},\mathbf{p}'} V_p^2 S(\mathbf{p}-\mathbf{p}')S(\mathbf{p}+\mathbf{p}') \\ &\quad \times [\Delta R_{\mathbf{p}}(E)]^2 \Delta R_{\mathbf{p}'}(E). \end{aligned} \quad (24)$$

The summation of \mathbf{q} in Eq. (23) has an upper cutoff q_c which is proportional to the inverse of the mean free path l_E ; i.e., $q_c = x_0 \pi / l_E$, where the arbitrary constant x_0 is believed to be of order unity. If we use the transport mean free path l_E^{tr} which is defined as

$$l_E^{\text{tr}} = \frac{3D_{BA}(E)}{V_E}, \quad (25)$$

the mobility edge E_c in $d=3$ is then determined by the relation

$$1 = \frac{\beta(E_c)}{N} \sum_{\mathbf{q}}' \frac{1}{q^2} \cong \frac{\beta(E_c) V_{E_c} x_0 a^3}{6\pi D_{BA}(E_c)}. \quad (26)$$

The reason that l_E^{tr} of Eq. (25) is called the transport mean free path is because of the presence of an equivalent term $(V_p^2 - \mathbf{V}_p \cdot \mathbf{V}_{p'})$ in $D_{BA}(E)$ of Eq. (20) which accounts for the momentum change along the direction of initial propagation.²¹ Alternatively, the single-particle mean free path l_E^s can be defined from the relaxation of the single-particle propagator.^{8,21,22} However, these two definitions of the mean free path will not give any qualitatively different physical results if the correlations are short range.²³ Here, for the case of electrons, only the transport mean free path of Eq. (25) will be used in the theory.

III. PHASE DIAGRAMS NEAR THE BAND-EDGE REGION AND QUASIUNIVERSALITY

In this section we will take the binary alloys as an example to study the effect of short-range correlations to the mobility edge in the near-band-edge region. Since only the correlation effect is of interest, we consider here

the simple case of equal concentrations of A and B atoms ($c=0.5$) with the site energies $\epsilon_A = W$ and $\epsilon_B = -W$ to avoid the band asymmetry and the appearance of the impurity states in the dilute limits. The correlation is introduced by a parameter α which is defined as the probability P_{AA} that a given nearest-neighbor (NN) of an A atom be an A atom. The probability P_{BA} that a given NN of an A atom be a B atom is then $P_{BA} = 1 - P_{AA} = 1 - \alpha$. We also have $P_{AB} = P_{BA}$ and $P_{BB} = 1 - P_{AB}$. When $\alpha = c = 0.5$, the alloy is completely random. The alloy has the clustering (or anticlustering) property when α is greater (or smaller) than 0.5. In $d=1$, once the NN correlation is defined, the correlation function between any two sites is determined uniquely so long as there are no multisite correlations in the system. This is not true in a three-dimensional lattice. For instance, due to the existence of loops, the next-nearest-neighbor (NNN) correlation cannot be determined from the NN correlation alone. To avoid more than one parameter in the problem, for simplicity, here we use the tree approximation for NNN correlation and set all the correlations beyond NNN to be zero. This is a good approximation if the correlation strength $\bar{\alpha} = \alpha - 0.5$ is small. The probability $P_{AA}^{(2)}$ that a given NNN of an A atom be an A atom becomes

$$P_{AA}^{(2)} = P_{AA} P_{AA} + P_{AB} P_{BA} = \alpha^2 + (1-\alpha)^2, \quad (27)$$

and

$$P_{BA}^{(2)} = 1 - P_{AA}^{(2)} = 2\alpha(1-\alpha).$$

With the above approximation, the correlation function becomes

$$\begin{aligned} \langle \epsilon_i \epsilon_j \rangle &= 0.5 \epsilon_A (P_{AA} \epsilon_A + P_{BA} \epsilon_B) \\ &\quad + 0.5 \epsilon_B (P_{BB} \epsilon_B + P_{AB} \epsilon_A) = (2\alpha - 1) W^2, \end{aligned} \quad (28)$$

$$\langle \epsilon_i \epsilon_k \rangle = (2\alpha - 1)^2 W^2 \quad \text{and} \quad \langle \epsilon_i \epsilon_l \rangle = 0,$$

where (i,j) , (i,k) , and (i,l) are, respectively, the NN, NNN, and beyond NNN pairs. From Eq. (4), the structure function $S(\mathbf{q})$ can be obtained. The SCBA is valid when both W and $\bar{\alpha}$ are small. In the near-band-edge region, the typical wavelength is much greater than the lattice constant a and we can approximate Eq. (5) and the $S(\mathbf{q})$ by

$$\epsilon(\mathbf{p}) \cong -6t + \frac{p^2}{2m^*}, \quad m^* = (2ta^2)^{-1}, \quad (29)$$

$$S(\mathbf{q}) \cong S(0) - S_2 q^2 a^2, \quad (30)$$

with

$$\begin{aligned} S(0) &= 1 + 6(2\alpha - 1) + 12(2\alpha - 1)^2, \\ S_2 &= (2\alpha - 1)(8\alpha - 3). \end{aligned} \quad (31)$$

Using the above approximations, all the averaged physical quantities become isotropic and all the momentum summations in Sec. II can be replaced by integrations.

To calculate the phase diagram, we take t as the energy scale and a as the length scale or equivalently $t = a = 1$. For the given small W and $\bar{\alpha}$, using Eqs. (29) and (30), the SCBA's of Eqs. (2) and (3) are solved numerically for $\Sigma_p^\pm(E)$ and $R_p^\pm(E)$. The momentum integration is cut off at $p_0 = \sqrt{3}\pi/2a$. Using the calculated $\Delta R_p(E)$, the corresponding $\rho(E)$, V_E^2 , $D_{BA}(E)$, and $\beta(E)$ can be evaluated using Eqs. (11), (13), (20), and (24), respectively. The mobility edge E_c is then determined from Eq. (26). We have taken the arbitrary constant x_0 to be 1. The phase diagrams in the near-band-edge region are shown in Fig. 2 for $\bar{\alpha} = \alpha - 0.5 = 0, 0.1, 0.2, 0.3, \text{ and } 0.4$ where the dimensionless energy scales are used for W and E . We do not consider the case of negative $\bar{\alpha}$ here. A negative $\bar{\alpha}$ gives two length scales, a and the correlation length, to the problem which cannot be adequately described by the approximated $S(\mathbf{q})$ of Eq. (30).²⁰ Also, due to the truncation introduced in Eq. (28), a negative $\bar{\alpha}$ may lead to a negative $S(0)$ or negative correlation length which is unphysical. It is worth noting that the dependence of the localization length on $\bar{\alpha}$ has been studied by various methods in $d = 1$ for both positive and negative $\bar{\alpha}$.^{15,16} In the case of complete randomness $\bar{\alpha} = 0$, the mobility edge curve shown in Fig. 2 is not inconsistent with the finite-size scaling result of Ref. 6 for $W/t \lesssim 1$. Comparing to the case $\bar{\alpha} = 0$, when $\bar{\alpha} > 0$, the mobility edge curve first shifts to the lower energies for small W/t and then bends over to higher energies as W/t is increased. The crossover value of W , $W_c(\bar{\alpha})$, is a decreasing function of $\bar{\alpha}$. This correlation-dependent crossover behavior will become transparent in the following discussions. First, we analyze the effect of the correlations to the phase diagram

in the long-wavelength limit. In the presence of the correlations, the scattering strength of the disordered potential is determined not only by the variance W^2 but also by the correlation function $C(\mathbf{R}_i - \mathbf{R}_j)$. In the limit when the characteristic length which is about $1/(\text{typical } p)$ is much greater than the correlation length, the problem is reduced to the WNM with $W^2 S(0)$ as the effective scattering strength. As defined in Eq. (4), $S(0)$ is the effective number of sites within the correlation range and is related to the correlation length L by $S(0)a^3 \approx L^3$. In this limit, it has been proposed²⁰ and shown in some cases^{22,24} that the physical quantities follow universal behaviors by choosing the proper energy scale ϵ_{03} and length scale L_{03} and shifting the origin of the energy to the nonuniversal band edge. It will be interesting to see if the mobility edge curves shown in Fig. 2 follow such a quasiuniversal behavior in the long-wavelength limit. Using the definitions of $\gamma = W^2 S(0)a^3$ and $\hbar^2/2m^* = a^2 t$ given in Ref. 20, ϵ_{03} and L_{03} are found to be $W^4 S^2(0)/t^3$ and $t^2 a / W^2 S(0)$, respectively. Since the left-handed side of the mobility equation (26) is a dimensionless constant, if the quasiuniversality holds, we would expect that the shifted and renormalized mobility edge $\bar{E}_c = [E_c(W, \bar{\alpha}) - E_b(W, \bar{\alpha})]/\epsilon_{03}$ be a constant value in the WNM limit where E_c and E_b are, respectively, the mobility edge and the band edge. In Fig. 3 we have replotted the mobility edge curves of Fig. 2 using the new energy scale \bar{E}_c . Indeed the scaling is seen and the universal value for mobility edge is about 0.019. This universal value depends on the choice of the arbitrary constant x_0 in Eq. (26) as will be seen explicitly in the later discussions. Figure 3 also shows that the scaling region in W space is systematically suppressed as $\bar{\alpha}$ is increased. This can be easily understood from the idea of effective scattering strength $W^2 S(0)$ which suggests that the re-

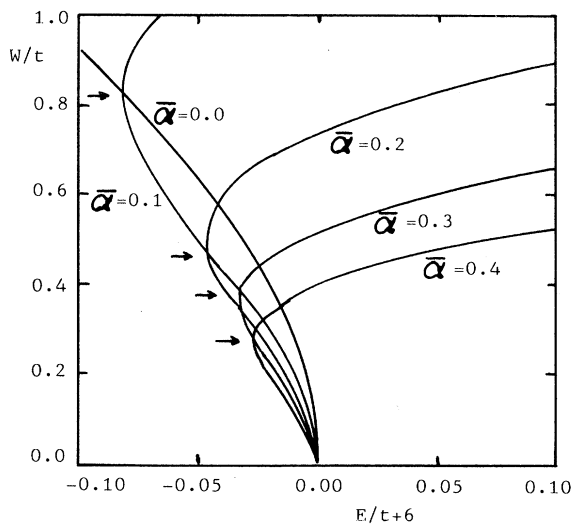


FIG. 2. The mobility edge curves which separate the localized region (left region of the curve) from the extended region (right region of the curves) for $\bar{\alpha} = 0, 0.1, 0.2, 0.3, \text{ and } 0.4$. The arrows show the crossover values, $W_c(\bar{\alpha})/t$.

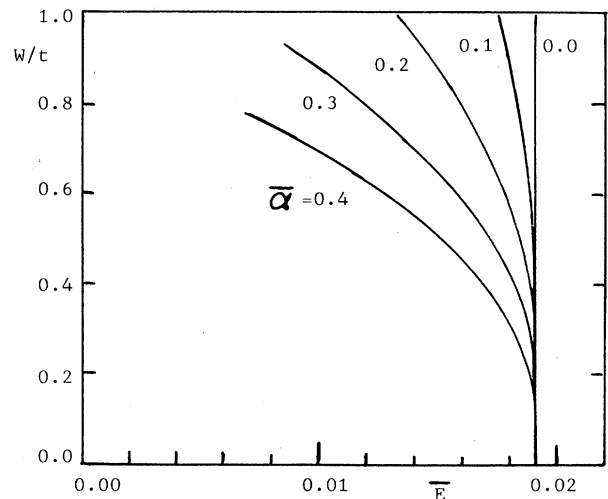


FIG. 3. The mobility edge curves of Fig. 2 are replotted using the shifted and renormalized energy scale \bar{E} for $\bar{\alpha} = 0, 0.1, 0.2, 0.3, \text{ and } 0.4$. Inside the scaling region, the mobility edge curves assume a constant universal value of 0.019.

gion in the W space where the WNM is valid is proportional to $1/\sqrt{S(0)}$, which is a decreasing function of $\bar{\alpha}$ according to Eq. (31). Outside the scaling region, the concept of effective scattering strength breaks down and the mobility edge depends on W and $\bar{\alpha}$ independently.

In the WNM limit, the mobility edge can be studied analytically using the following procedure without solving the SCBA of Eqs. (2) and (3). By writing $R_p^+(E)$ of Eq. (2) as $[E + 6t - \tau_p(E) - i\gamma_p(E) - p^2/2m^*]^{-1}$, in the limit when W and $\bar{\alpha}$ are small, $\text{Im}R_p^+(E)$ can be approximated by $-\pi\delta[E + 6t - \tau_p(E) - p^2/2m^*]$. For a given energy E , let us define the typical p as the value such that $E + 6t - \tau_p(E) - p^2/2m^* = 0$. By using the above approximation, we can express all the physical quantities in terms of the typical p without knowing $\tau_p(E)$ explicitly. By calculating the approximated band edge E_b using Eq. (3) and the typical p_c at the mobility edge using Eq. (26), the mobility edge E_c can be taken as $E_b + p_c^2/2m^*$. Since the typical p at the band edge is $p = 0$, from the function $\gamma_p(E_b) = 0$ and Eq. (3) we have

$$E_b \cong -6t + \tau_0(E_b), \quad (32)$$

and

$$\begin{aligned} \tau_0(E_b) &\cong \frac{W^2 a^3}{(2\pi)^3} \int_0^{p_0} d\mathbf{p}' \text{Re} \left[\frac{S(p')}{\tau_0(E_b) - \tau_{p'}(E_b) - \frac{p'^2}{2m^*}} \right] \\ &\cong \frac{-W^2 m^* a^3 p_0}{3\pi^2} [3S(0) - S_2 a^2 p_0^2], \end{aligned} \quad (33)$$

where S_2 is given by Eq. (31). In Eq. (33) we have approximated $\tau_p \approx \tau_0$, which is valid in the small $\bar{\alpha}$ limit. Using the δ -function approximation for $\Delta R_p(E)$, Eqs. (11), (13), (20), and (24) can be evaluated, yielding

$$\rho(E) \cong \frac{m^* a^3 p}{2\pi^2}, \quad (34)$$

$$V_E \cong p/m^*, \quad (35)$$

$$D_{\text{BA}}(E) \cong \frac{\pi p}{a^3 m^* W^2 [3S(0) - 8S_2 p^2 a^2]}, \quad (36)$$

and

$$\beta(E) \cong \frac{2m^* W^2 [3S^2(0) - 12S(0)S_2 p^2 a^2 + 8S_2^2 p^4 a^4]}{p^2 [S(0) - 2S_2 p^2 a^2]}. \quad (37)$$

Substituting Eqs. (35)–(37) into Eq. (26), p_c is then determined. In the WNM limit, by keeping only the leading terms in p_c , Eq. (26) gives

$$1 = 3x_0 a^8 \left[\frac{m^* W^2 S(0)}{\pi p_c a} \right]^2. \quad (38)$$

From Eqs. (32), (33), and (38) and using the relation $2m^* = (ta^2)^{-1}$, the mobility edge E_c becomes

$$\begin{aligned} \frac{E_c}{t} &\cong -6 - \frac{p_0 a}{6\pi^2} [3S(0) - S_2 a^2 p_0^2] \left[\frac{W}{t} \right]^2 \\ &\quad + \frac{3x_0 S^2(0)}{16\pi^2} \left[\frac{W}{t} \right]^4. \end{aligned} \quad (39)$$

With the values of $p_0 = \sqrt{3}\pi/2a$ and $x_0 = 1$ used in the numerical calculations, E_c/t of Eq. (39) gives very good agreement with the curves shown in Fig. 2 in the region below the crossover value $W_c(\bar{\alpha})/t$. Thus the phase diagrams shown in Fig. 2 can be understood as follows. When W/t is small, the shift of the mobility edge toward lower energies follows essentially the shift of the band edge which is of order $(W/t)^2$. When W/t is increased, the coherent backscattering effect which is of order $(W/t)^4$ tends to bend the mobility edge toward higher energies. It is the competition of these two effects which gives the crossover behavior shown in Fig. 2. The coefficients of the terms $(W/t)^2$ and $(W/t)^4$ in Eq. (39) give the correlation dependence of the crossover values $W_c(\bar{\alpha})/t$ which is not inconsistent with the results shown in Fig. 2. In the limit when p_c is small, from Eqs. (25), (35), (36), and (38), we have

$$l_E^{\text{lr}}(E_c) \cong \frac{4a}{S(0)} \left[\frac{t}{W} \right]^2, \quad (40)$$

and

$$p_c \cong \frac{\sqrt{3x_0 S(0)}}{4\pi a} \left[\frac{W}{t} \right]^2. \quad (41)$$

Thus the Ioffe-Regel constant $p_c l_E$ for the localization is a constant ($=\sqrt{3x_0}/\pi$) in the WNM limit which is independent of the correlations and has the value 1.732 when $x_0 = 1$. In fact, our numerical calculations show that outside the scaling region the value of $p_c l_E$ is always in the range ~ 1.73 – 1.80 ; even the value of p_c has been increased by more than an order of magnitude. In the WNM limit, we would expect that all the physical quantities follow quasiuniversal behaviors. Using the energy and length scales, $\epsilon_{03} = W^4 S^2(0)/t^3$ and $L_{03} = t^2 a / W^2 S(0)$, found earlier, the dimensionless functions of $\rho(E)$, V_E , $D_{\text{BA}}(E)$, and $\beta(E)a^3$ of Eqs. (34)–(37) can be expressed by the following universal functions of the shifted and scaled variable \bar{E} :

$$L_{03}^3 \epsilon_{03} \rho(E) a^{-3} \cong (\bar{E})^{1/2} / 4\pi^2, \quad (42)$$

$$(L_{03} \epsilon_{03})^{-1} V_E \cong 2(\bar{E})^{1/2}, \quad (43)$$

$$(L_{03}^2 \epsilon_{03})^{-1} D_{\text{BA}} \cong \frac{8\pi}{3} (\bar{E})^{1/2}, \quad (44)$$

and

$$L_{03}^{-1} \beta(E) a^3 \cong \frac{3}{2} \frac{1}{\bar{E}} \quad (45)$$

with

$$\bar{E} = \frac{E - E_b}{\epsilon_{03}} \cong \frac{p^2 a^2 t^4}{W^4 S^2(0)}. \quad (46)$$

In the WNM limit, we would also expect that the scaling shown in Fig. 3 holds exactly. With the use of Eq. (39), we find immediately that the universal mobility edge constant $\bar{E}_c = (E_c - E_b)/\varepsilon_{03} \cong 3x_0/16$ which has the value 0.019 shown in Fig. 3 when x_0 is taken to be 1.

IV. FORMULATION FOR PHONONS

Consider a d -dimensional hypercubic harmonic mixed crystal with random masses m_i but constant isotropic force constant K between NN sites. The equations of motion, in the frequency space, for the displacement u_i along any direction of the lattice have the form

$$(2dk - m_i E^2)u_i = (2dk - \bar{m}E^2 - \Delta m_i E^2)u_i = K \sum_l' u_l, \quad (47)$$

where the summation of l is over all the NN sites of i , $\bar{m} = \langle m_i \rangle$ is the averaged mass, and E is now the frequency of the phonons. In the absence of the correlations, the localization properties of the three-dimensional binary systems have been studied by the authors using the theory of VW in conjunction with the CPA.¹³ In the presence of the correlations, it is not known how to incorporate the CPA into the theory of VW. Here we will formulate the problem in the SCBA. The correlation function for the disordered mass $\Delta m_i (= m_i - \bar{m})$ can be denoted as $\langle \Delta m_i \Delta m_j \rangle = \gamma^2 C(\mathbf{R}_i - \mathbf{R}_j)$ where γ^2 is the variance of the mass distribution $P(m_i)$. From the similarity between the equations of motion for the electrons with Hamiltonian Eq. (1) and the phonons of Eq. (47), it is easy to see that the averaged single-phonon Green's function in the SCBA is given by

$$R_{\mathbf{p}}^{\pm}(E) = [(\bar{m}E^2 - \bar{\varepsilon}(\mathbf{p}) - \Sigma_{\mathbf{p}}^{\pm}(E))]^{-1}, \quad (48)$$

$$\Sigma_{\mathbf{p}}^{\pm}(E) = \frac{\gamma^2 E^4}{N} \sum_{\mathbf{p}'} S(\mathbf{p} - \mathbf{p}') R_{\mathbf{p}'}^{\pm}(E), \quad (49)$$

$$S(\mathbf{q}) = \sum_i C(\mathbf{R}_i) e^{i\mathbf{q} \cdot \mathbf{R}_i}, \quad (50)$$

and

$$\bar{\varepsilon}(\mathbf{p}) = K \left[2d - \sum_{\delta} e^{i\mathbf{p} \cdot \delta} \right]. \quad (51)$$

Like the case of electrons, the transport and localization properties for phonons are related to the averaged two-phonon Green's function $\phi_{\mathbf{p}, \mathbf{p}'}^E(\mathbf{q}, \omega)$ which has the same form as Eq. (6) for the electrons.¹³ With the use of Eq. (48), the Bethe-Salpeter equation also has the same form as given in Eqs. (7)–(9) except that the first term ω in Eq. (7) is replaced by $2E\bar{m}\omega$. From now on, the derivations of the bare and renormalized diffusion constants, $D_{\text{BA}}(E)$ and $D(E)$, are completely parallel to the case of electrons. Here we will simply write down the following results:

$$D_{\text{BA}}(E) = \frac{-iV_E^4 \Delta R_{ii}(E)}{2\bar{m}E^5 d^2 \gamma^2} \times \left[\frac{1}{N^2} \sum_{\mathbf{p}_1, \mathbf{p}_2} \Delta R_{\mathbf{p}_1}(E) S(\mathbf{p}_1 - \mathbf{p}_2) \Delta R_{\mathbf{p}_2}(E) \times (\mathbf{V}_{\mathbf{p}_1} \cdot \hat{\mathbf{q}})(\mathbf{V}_{\mathbf{p}_1} - \mathbf{V}_{\mathbf{p}_2}) \cdot \hat{\mathbf{q}} \right]^{-1}, \quad (52)$$

$$\frac{V_E^2}{d} = \frac{1}{N} \sum_{\mathbf{p}} (\mathbf{V}_{\mathbf{p}} \cdot \hat{\mathbf{q}})^2 \Delta R_{\mathbf{p}}(E) / \Delta R_{ii}(E), \quad (53)$$

$$\beta(E) = \frac{-d\gamma^4 E^8}{\Delta R_{ii}(E) V_E^4} \frac{1}{N^2} \sum_{\mathbf{p}_1, \mathbf{p}_2} V_{\mathbf{p}_1}^2 S(\mathbf{p}_1 - \mathbf{p}_2) S(\mathbf{p}_1 + \mathbf{p}_2) \times [\Delta R_{\mathbf{p}_1}(E)]^2 \Delta R_{\mathbf{p}_2}(E), \quad (54)$$

and

$$D(\omega, E) = D_{\text{BA}}(E) \left[1 - \frac{\beta(E)}{N} \sum_{\mathbf{q}}' \frac{1}{q^2 - i\omega/D(\omega, E)} \right], \quad (55)$$

with

$$\mathbf{V}_{\mathbf{p}} = \frac{\partial \bar{\varepsilon}(\mathbf{p})}{\partial \mathbf{p}}, \quad \Delta R_{ii}(E) = \frac{1}{N} \sum_{\mathbf{p}} \Delta R_{\mathbf{p}}(E), \quad (56)$$

where $R_{ii}(E) = \langle G_{ii}(E) \rangle$ is the averaged diagonal Green's function in the site representation. As discussed in Ref. 13, the group velocity of the phonons $V_{\mathbf{q}}$, which is not the V_E given in Eq. (53), can be defined as

$$V_{\mathbf{q}}^2(E) = \frac{-1}{2\pi E \bar{m} \rho_{\text{ph}}(E)} \frac{1}{N} \sum_{\mathbf{p}} V_{\mathbf{p}}^2 \text{Im} R_{\mathbf{p}}^+(E), \quad (57)$$

where $\rho_{\text{ph}}(E)$ is the phonon density of states and is given by

$$\rho_{\text{ph}}(E) = \frac{-2E}{\pi} \text{Im} \langle m_i G_{ii}^+(E) \rangle \cong \frac{iE\bar{m}}{\pi} \Delta R_{ii}(E). \quad (58)$$

The transport mean free path used for the cutoff q_c in Eq. (55) becomes

$$l_E^{\text{tr}} = \frac{3D_{\text{BA}}(E)}{V_{\mathbf{q}}(E)}. \quad (59)$$

The above equations are valid in the low-frequency region where the scattering is weak. Since the phonons are extended in this region when $d=3$, we will only study the localization properties for $d=1$ and 2 in the next section. In the absence of a better theory, even outside the region of validity of the SCBA, the equations given in this section may also provide a method to investigate qualitatively the effect of the correlations to the transport and localization properties of the phonons in the whole frequency band as it does for the case of the electrons.^{15,19}

V. LOCALIZATION BEHAVIORS IN $d=1$ AND 2 AND UNIVERSALITY

A. General results for small E

In the long-wavelength limit, the equations given in the last section can be much simplified. The function $\bar{\varepsilon}(\mathbf{p})$ of

Eq. (51) can be approximated by Ka^2p^2 and all the momentum summations can be replaced by integrations with a suitable upper cutoff p_0 . As we will see later, in the weak scattering limit, the value of p_0 is irrelevant. Here, we consider the following two kinds of correlations:

$$C(\mathbf{R}_i - \mathbf{R}_j) = e^{-|\mathbf{R}_i - \mathbf{R}_j|/a\alpha}, \quad (60)$$

$$C(\mathbf{R}_i - \mathbf{R}_j) = \frac{(\alpha a)^{2n}}{(|\mathbf{R}_i - \mathbf{R}_j|^2 + \alpha^2 a^2)^n}. \quad (61)$$

Again, the above correlation functions are normalized to $C(0)=1$. These forms of the correlations have been used in Ref. 14 for the continuous medium which can be obtained by letting $a \rightarrow 0$ and $\alpha \rightarrow \infty$ while keeping $a\alpha$ constant. Here we only require that α be sufficiently large so that the lattice summation in Eq. (50) can be approximated by an integration. In Ref. 14, the asymptotic behaviors of the wave localization in a continuum have been studied by using the replica method in conjunction with the CPA (or SCBA) in $d=1$ and 2.¹⁴ Here we will study this problem independently using the theory of VW to obtain the complete expressions for the localization length. However, some of the results of Ref. 14 are quite useful and will be quoted here.

With the above considerations, Eqs. (48)–(50) can be simplified as

$$R_p^\pm(E) = [\bar{m}(E^2 - \bar{c}^2 p^2) \mp i\gamma_p(E)]^{-1}, \quad (62)$$

$$\gamma_p(E) = \gamma^2 E^4 \left[\frac{a}{2\pi} \right]^d \int_{p' < p_0}^{d p'} \frac{S(|\mathbf{p} - \mathbf{p}'|) \gamma_{p'}(E)}{[\bar{m}(E^2 - \bar{c}^2 p'^2)]^2 + \gamma_{p'}^2(E)}, \quad (63)$$

$$S(q) = \frac{1}{a^d} \int d\mathbf{R} C(\mathbf{R}) e^{i\mathbf{q} \cdot \mathbf{R}}, \quad (64)$$

where $\bar{c}^2 = Ka^2/\bar{m}$ and the function $\gamma_p(E)$ is the imaginary part of the self-energy $\Sigma_p^+(E)$ and is negative according to our definition. It can be shown that the real part of $\Sigma_p^+(E)$ is of order $E^{2+\Delta}$ with $\Delta > 0$ for all the correlations considered in Eqs. (60) and (61) and thus can be ignored. With the use of Eqs. (62) and (63), it will be shown in the Appendix that the expressions for $D_{BA}^{(E)}$, V_E , $\beta(E)$, V_g , and $\rho_{ph}^{(E)}$ of Eqs. (52)–(54), (57), and (58) reduce to

$$V_E^2 \cong 4\bar{m}^2 E^2 \bar{c}^2, \quad V_g(E) \cong \bar{c}, \quad (65)$$

$$\rho_{ph}(E) \cong \frac{a^d}{E} \left[\frac{E}{2\pi\bar{c}} \right]^d \int d\Omega \hat{\Omega}^p, \quad (66)$$

$$D_{BA}(E) \cong -\frac{2\pi\rho_{ph}(E)}{dE^2\gamma^2} \left[\frac{2\pi}{a} \right]^{2d} \times \left[\int_{p_1, p_2 < p_0} d\mathbf{p}_1 d\mathbf{p}_2 \Delta R_{p_1}(E) \times S(|\mathbf{p}_1 - \mathbf{p}_2|) \Delta R_{p_2}(E) (p_1^2 - \mathbf{p}_1 \cdot \mathbf{p}_2) \right]^{-1}, \quad (67)$$

and

$$\beta(E) \cong -\frac{dr_p(E)}{\pi\bar{m}\bar{c}^2 E \rho_{ph}(E)}, \quad (68)$$

where $\int d\Omega_{\hat{p}}$ represents the summation of the unit vectors \hat{p} and $-\hat{p}$ in $d=1$ and the integration of the angular variable in $d=2$. The momentum p of $\gamma_p(E)$ in Eq. (68) is the typical momentum, i.e., $p = E/\bar{c}$. In the localized region, the diffusion constant $D(\omega, E)$ of Eq. (55) is related to the localization length $\xi_l(E)$ by $D(\omega, E) \cong -i\omega\xi_l^2(E)$.⁷ Substituting this relation into Eq. (55), we find

$$1 \cong \beta(E) \left[\frac{a}{2\pi} \right]^d \int d\Omega \hat{\Omega} \int_0^{q_c} \frac{q^{d-1} dq}{q^2 + \xi_l^{-2}(E)}, \quad q_c = \frac{\pi x_0}{l_E}, \quad (69)$$

where the function $\beta(E)$ is given by Eq. (68). If the transport mean free path is used, we have, from Eqs. (59) and (65),

$$l_E^{\text{tr}} \cong \frac{3D_{BA}(E)}{\bar{c}}. \quad (70)$$

Alternatively, we can define a single-phonon mean free path which, in the weak scattering limit, is related to the single-phonon relaxation time τ_E by $l_E^s = \bar{c}\tau_E$. By writing $[R_p^\pm(E)]^{-1}$ of Eq. (62) as $\bar{m}[(E \pm iy/\tau_E) - \bar{c}^2 p^2]$, and choosing $y = 3/2^d$, l_E^s becomes

$$l_E^s \cong \frac{-3E\bar{m}\bar{c}}{2^{d-1}\gamma_p(E)}. \quad (71)$$

This form of l_E^s can also be obtained from Eq. (70) if the term $(p_1^2 - \mathbf{p}_1 \cdot \mathbf{p}_2)$ in $D_{BA}(E)$ of Eq. (67) is replaced by p_1^2 .²¹ It is exactly this difference in the definitions of l_E^{tr} and l_E^s that leads to different asymptotic behaviors when the long-range correlations are present. Here we have deliberately chosen $y = 3/2^d$ to make the two mean free paths defined in Eqs. (70) and (71) identical when the correlations are short range so that their difference will be more transparent when the long-range correlations are considered. For any given correlation function, the problem now is to find the explicit forms for $\gamma_p(E)$ and $D_{BA}(E)$ from Eqs. (63) and (67) and solve Eq. (69) for $\xi_l(E)$.

B. Short-range correlations and universality

For the case of exponential correlations of Eq. (60) or the power-law correlations of Eq. (61) with $2n > d$, the correlation function $C(R)$ is integrable. By letting the argument of the structure function $S(q)$ be zero and using the δ -function approximation for $\text{Im}R_p(E)$ as described in the Appendix, Eqs. (63) and (67) can be integrated, yielding

$$\gamma_p(E) \cong \frac{-\gamma^2 S(0) E^2}{\bar{m}} \left[\frac{aE}{2\bar{c}} \right]^d, \quad (72)$$

$$D_{BA}(E) \cong -E\bar{m}\bar{c}^2/2^{d-1}\gamma_p(E), \quad (73)$$

where $d=1$ and 2. As mentioned before, from Eqs.

(70)–(73), we have $l_E^{\text{tr}} = l_E^s$. Substituting Eqs. (72) and (73) into Eq. (69) and using Eq. (68), we find the following results for:

$$\begin{aligned} \xi_l^{\text{tr}}(E) &= \xi_l^s(E) \cong \frac{2\bar{m}^2 \bar{c}^2 A}{\gamma^2 S(0) a E^2}, \\ A &= \frac{3}{x_0 \pi} \tan \left[\frac{\pi}{A} \right] \quad \text{for } d=1, \\ \xi_l^{\text{tr}}(E) &= \xi_l^s(E) \cong \frac{6\bar{m}^2 \bar{c}^3}{x_0 \pi \gamma^2 S(0) a^2 E^3} \exp \left[\frac{2\pi \bar{m}^2 \bar{c}^2}{\gamma^2 S(0) a^2 E^2} \right] \\ &\quad \text{for } d=2. \end{aligned} \quad (74)$$

Like the case of electrons, the effective scattering strength $\gamma^2 S(0)$ is the relevant disorder parameter. The straightforward integration of Eq. (64) gives (i) for exponential correlations, $S(0) = 2\alpha$ for $d=1$ and $S(0) = 2\pi\alpha^2$ for $d=2$, and (ii) for power-law correlations with $2n > d$, $S(0) = \sqrt{\pi} \alpha \Gamma(n - \frac{1}{2}) / \Gamma(n)$ for $d=1$ and $S(0) = \pi\alpha^2 / (n-1)$ for $d=2$ where $\Gamma(n)$ is the Γ function. In order to see the scaling behavior, we follow the same procedure as given in Ref. 20. The reduction of Eq. (47) to the WNM gives the usual wave equation with the δ -correlation function in the mass density. It can be shown that the natural units ε_{0d} for the product of the mass and the frequency squared and L_{0d} for the length are related to the parameters of the original problem by

$$\varepsilon_{0d} L_{0d}^2 = \bar{m} \bar{c}^2 = K a^2, \quad (76)$$

$$\varepsilon_{0d}^2 L_{0d}^{d+4} = \gamma^2 S(0) \bar{c}^4 a^d, \quad (77)$$

which give

$$L_{0d} = \left[\frac{\gamma^2 S(0)}{\bar{m}^2} \right]^{1/d} a, \quad (78)$$

$$\varepsilon_{0d} = \frac{\bar{m} \bar{c}^2}{a^2} \left[\frac{\bar{m}^2}{\gamma^2 S(0)} \right]^{2/d}, \quad (79)$$

$$E_{0d} = \frac{\bar{c}}{a} \left[\frac{\bar{m}^2}{\gamma^2 S(0)} \right]^{1/d}, \quad (80)$$

where $E_{0d} (= \bar{c} / L_{0d})$ is the natural unit for the frequency. Using the renormalized scale $\bar{E} = E / E_{0d}$, the dimensionless functions of γ_p , D_{BA} , and ξ_l given in Eqs. (72)–(75) become

$$\varepsilon_{0d}^{-1} \gamma_p(E) \cong -\bar{E}^{2+d} / 2^d, \quad (81)$$

$$L_{0d}^2 E_{0d} D_{\text{BA}}(E) \cong 2 / \bar{E}^{(1+d)}, \quad (82)$$

$$L_{0d}^{-1} \xi_l(E) \cong \begin{cases} 2A / \bar{E}^2, & d=1 \\ \frac{6}{x_0 \pi} \frac{1}{\bar{E}^3} \exp \left[\frac{2\pi}{\bar{E}^2} \right], & d=2. \end{cases} \quad (83)$$

Also, from Eqs. (66) and (68), we have

$$L_{0d}^d E_{0d} \rho(E) a^{-d} \cong \frac{1}{\pi} \left[\frac{\bar{E}}{2} \right]^{d-1}, \quad (84)$$

$$L_{0d}^{2-d} \beta(E) a^d \cong \bar{E}^2 / 2^{(d-2)}. \quad (85)$$

The results of Eqs. (81)–(84) are consistent with the known result.¹⁴

C. Long-range correlations

When $2n \leq d$, the correlation function of Eq. (61) is nonintegrable and the structure function $S(|\mathbf{p}-\mathbf{p}'|)$ becomes singular when $\mathbf{p}=\mathbf{p}'$. It has been shown in Appendix A of Ref. 14 that when $1 < 2n < 2$ in $d=2$ the angular integration of the structure function in Eq. (63), i.e., $\int d\Omega_{\mathbf{p}} S(|\mathbf{p}-\mathbf{p}'|)$, converges so long as p and p' are finite and the δ -function approximation can still be used for $\text{Im}R_p(E)$. However, when $2n < 1$ (for both $d=1$ and 2) the angular integration of the structure function gives a singular function of $|p-p'|$ and the δ -function approximation is no longer self-consistent. In this case, one has to solve Eq. (63) self-consistently for the $\gamma_p(E)$. Once $\gamma_p(E)$ is known, the single-phonon localization length ξ_l^s is obtained from Eqs. (69) and (71). However, for the transport ξ_l^{tr} , we have to evaluate $D_{\text{BA}}(E)$ from Eq. (67). Since $S(|\mathbf{p}_1-\mathbf{p}_2|)$ is singular at $\mathbf{p}_1=\mathbf{p}_2$, the presence of the term $p_1^2 - \mathbf{p}_1 \cdot \mathbf{p}_2$ in Eq. (67) becomes extremely important in the cancellation of the singularity in $S(|\mathbf{p}_1-\mathbf{p}_2|)$. The effect of the term $p_1^2 - \mathbf{p}_1 \cdot \mathbf{p}_2$ in $D_{\text{BA}}(E)$ is to enhance the relaxation time and to increase the mean free path and localization length. Thus we would expect that $l_E^{\text{tr}} \geq l_E^s$ and $\xi_l^{\text{tr}} \geq \xi_l^s$ in general. In fact, we have found that the angular integration of the function $S(|\mathbf{p}_1-\mathbf{p}_2|)(p_1^2 - \mathbf{p}_1 \cdot \mathbf{p}_2)$ converges for all $2n \leq d$ and the δ -function approximation can be used for ΔR_{p_1} and ΔR_{p_2} in Eq. (67). Since the calculations are quite lengthy and tedious, here we will only present the results of the calculations.

For $d=1$, the following results are obtained to the leading order in E .

(a) $n = \frac{1}{2}$:

$$\gamma_p(E) \cong \frac{3\gamma^2}{2\bar{m}} E^2 \omega \ln \omega, \quad (86)$$

$$D_{\text{BA}}(E) \cong \frac{-\bar{m} \bar{c}^2}{\gamma^2 E \omega \ln \omega}, \quad (87)$$

$$\frac{l_E^s}{\alpha a} = \frac{2}{3} \frac{l_E^{\text{tr}}}{\alpha a} \cong \frac{-2\bar{m}^2}{\gamma^2 \omega^2 \ln \omega}, \quad (88)$$

$$\frac{\xi_l^s(E)}{\alpha a} = \frac{A}{A'} \frac{\xi_l^{\text{tr}}(E)}{\alpha a} = \frac{-2\bar{m}^2 A}{3\gamma^2 \omega^2 \ln \omega}, \quad (89)$$

$$A' = \frac{9}{2x_0 \pi} \tan \left[\frac{\pi}{A'} \right],$$

where A is given by Eq. (74) and $\omega = E\alpha a / \bar{c}$ is the dimensionless frequency. Comparing to Eq. (80) of the short-range case, the scaling of the frequency does not contain the mass fluctuations. Since $A' > A$ is independent of x_0 , we have $\xi_l^{\text{tr}} > \xi_l^s$ as expected. In this case ξ_l^{tr} and ξ_l^s have

the same asymptotic forms.

(b) $0 < n < \frac{1}{2}$:

$$\gamma_p(E) \cong -F_1(n) \left[\frac{\gamma^2}{\bar{m}} \right]^{1/[2(1-n)]} \bar{m} E^2 \omega^{n(1-n)}, \quad (90)$$

$$D_{BA}(E) \cong \frac{\bar{m}^2 \bar{c}^2}{G_1(n) \gamma^2 E \omega^{2n}}, \quad (91)$$

$$\frac{\xi_l^{\text{tr}}(E)}{\alpha a} \cong \left[\frac{3}{x_0 F_1(n) G_1(n)} \right]^{1/2} \left[\frac{\bar{m}^2}{\gamma^2} \right]^{(3-2n)/[4(1-n)]} \times \omega^{(2n^2-n-2)/[2(1-n)]}, \quad (92)$$

$$\frac{\xi_l^s(E)}{\alpha a} \cong \frac{A}{F_1(n)} \left[\frac{\bar{m}^2}{\gamma^2} \right]^{1/[2(1-n)]} \omega^{-1/(1-n)}, \quad (93)$$

with

$$F_1(n) = \left[\frac{\Gamma(n) \Gamma(1-n) \Gamma(1-2n) \sin(n\pi)}{\pi 4^n} \right]^{1/[2(1-n)]}, \quad (94)$$

and

$$G_1(n) = 2^{2n-1} \Gamma(1-2n) \sin(n\pi), \quad (95)$$

where A in Eq. (93) is given by Eq. (74). In this case, ξ_l^{tr} and ξ_l^s have different asymptotic behaviors. Since the relation $0 < n < \frac{1}{2}$ implies $2+n-2n^2 > 2$, by comparing the exponents of ω in Eqs. (92) and (93), we have $\xi_l^{\text{tr}}/\xi_l^s \rightarrow \infty$ as $\omega \rightarrow 0^+$.

For $d=2$, the following four different behaviors are obtained for $2n < d=2$.

(a) $n=1$:

$$\gamma_p(E) \cong \frac{\pi \gamma^2 E^2 \omega^2 \ln \omega}{2\bar{m}}, \quad (96)$$

$$D_{BA}(E) \cong \frac{-\bar{m}^2 \bar{c}^2}{\pi \gamma^2 E \omega^2 \ln \omega}, \quad (97)$$

$$\frac{\xi_l^s(E)}{\alpha a} = \frac{\xi_l^{\text{tr}}(E)}{\alpha a} \cong \frac{-3\bar{m}^2}{x_0 \pi^2 \gamma^2 \omega^2 \ln \omega} \exp \left[\frac{-\bar{m}^2}{\gamma^2 \omega^2 \ln \omega} \right]. \quad (98)$$

(b) $\frac{1}{2} < n < 1$:

$$\gamma_p(E) \cong \frac{-F_2(n) \gamma^2 E^2 \omega^{2n}}{\bar{m}}, \quad (99)$$

$$D_{BA}(E) \cong \frac{n \bar{m}^2 \bar{c}^2}{2(2n-1) F_2(n) \gamma^2 E \omega^{2n}}, \quad (100)$$

$$\frac{\xi_l^s(E)}{\alpha a} = \frac{2n-1}{n} \frac{\xi_l^{\text{tr}}(E)}{\alpha a} \cong \frac{3\bar{m}^2}{2x_0 \pi F_2(n) \gamma^2 \omega^{2n+1}} \exp \left[\frac{-\bar{m}^2}{2F_2(n) \gamma^2 \omega^{2n}} \right], \quad (101)$$

with

$$F_2(n) = -2^{2n-3} \Gamma(2-2n) \Gamma^2(n-\frac{1}{2}) \cos(n\pi) / \Gamma^2(n). \quad (102)$$

(c) $n = \frac{1}{2}$:

$$\gamma_p(E) \cong \frac{\gamma^2 E^2 \omega \ln \omega}{2\bar{m}}, \quad (103)$$

$$D_{BA}(E) \cong \frac{\bar{m}^2 \bar{c}^2}{2\gamma^2 E \omega}, \quad (104)$$

$$\frac{\xi_l^s(E)}{\alpha a} = \frac{-2}{\ln \omega} \frac{\xi_l^{\text{tr}}(E)}{\alpha a} \cong \frac{-3\bar{m}^2}{x_0 \pi \gamma^2 \omega^2 \ln \omega} \exp \left[\frac{-\pi \bar{m}^2}{\gamma^2 \omega \ln \omega} \right]. \quad (105)$$

(d) $0 < n < \frac{1}{2}$:

$$\gamma_p(E) \cong -F_3(n) \left[\frac{\gamma^2}{\bar{m}^2} \right]^{1/[2(1-n)]} \bar{m} E^2 \omega^{n/(1-n)}, \quad (106)$$

$$D_{BA}(E) \cong \frac{\bar{m}^2 \bar{c}^2}{G_3(n) \gamma^2 E \omega^{2n}}, \quad (107)$$

$$\begin{aligned} \frac{\xi_l^s(E)}{\alpha a} &= \left[\frac{G_3(n)}{2F_3(n)} \left[\frac{\bar{m}^2}{\gamma^2} \right]^{(2n-1)/[2(1-n)]} \right. \\ &\quad \times \omega^{[n(1-2n)]/(1-n)} \left. \right] \frac{\xi_l^{\text{tr}}(E)}{\alpha a} \\ &= \frac{3}{2x_0 \pi} \left[\frac{\bar{m}^2}{\gamma^2} \right]^{1/[2(1-n)]} \frac{1}{\omega^{1/(1-n)}} \\ &\quad \times \exp \left[\frac{\pi}{2F_3(n)} \left[\frac{\bar{m}^2}{\gamma^2} \right]^{1/[2(1-n)]} \frac{1}{\omega^{n/(1-n)}} \right], \end{aligned} \quad (108)$$

with

$$F_3(n) = \left[\frac{\Gamma(1-n) \Gamma(\frac{1}{2}-n)}{\sqrt{\pi} 2^{4n}} \right]^{1/(2-2n)}, \quad (109)$$

and

$$G_3(n) = \frac{\Gamma(1-n) [\sqrt{\pi} (1-n) \Gamma(\frac{1}{2}+n) - Q \Gamma(1+n)]}{\Gamma(n) \Gamma(n+1)}, \quad (110)$$

$$Q = (1-2n) \sum_{m=1}^{\infty} \frac{(2m-1)!!}{2^m m! (2m+2n-1)}. \quad (111)$$

Except the case $n=1$, ξ_l^{tr} is always greater than ξ_l^s for $0 < n < 1$ and their difference lies only in the prefactor as can be seen from Eqs. (98), (101), (105), and (108).

VI. CONCLUSIONS AND DISCUSSIONS

The theory of VW is generalized in the context of the SCBA to include the correlations among the disordered potentials for both tight-binding electrons and phonons. Although the SCBA, in contrast to more elaborated theories such as the CPA, involves only the second moment of the distribution function P , it is correct when the

effective scattering strength $W^2S(0)$ is small in the electron case and in the long-wavelength limit of the phonon case where the scattering is weak. Outside the above regions of validity the SCBA still provides information concerning the effects of the correlations as has been demonstrated in the calculations of the one-dimensional electron case.¹⁵ How to incorporate a CPA-like approximation into the theory of VW when the correlations are present is still a challenging problem.

For the case of electrons in $d=3$, the phase diagrams for the binary alloys with short-range correlations are solved numerically near the band-edge region. The idea of quasiuniversality is confirmed and a scaling region is found in the W space. Inside the scaling region, the effective scattering strength $W^2S(0)$ is the only relevant disorder parameter. The effect of the correlations is found to suppress the scaling region in W space. Outside the scaling region the concept of the effective scattering strength breaks down and the mobility edge has to be described by W and the correlations independently.

For the case of phonons in $d=1$ and 2, the localization length and other physical quantities are studied analytically in the long-wavelength limit. When the correlations are short range, the effective scattering strength $\gamma^2S(0)$ also applies and the idea of universality holds as expected. In the presence of long-range correlations, different expressions for the localization length are obtained depending on the definitions of the mean free path used in the theory. Since the divergence of the structure function in the forward scattering angle does not contribute to the relaxation time in the transport sense, the transport localization length is generally greater than the single-phonon localization length which is obtained from the single-phonon relaxation time. In $d=1$, when $0 < n < \frac{1}{2}$, even the asymptotic behaviors are different. In $d=2$, the differences appear in the prefactors. All the expressions for the single-phonon localization length ξ_j^s obtained here give the same asymptotic behaviors found previously in Ref. 14 by using the replica method. In that work, the bare conductance $1/g_0^2 [\propto \rho_{\text{ph}}(E)D_{\text{BA}}(E)]$ used in the single-parameter scaling relation

$$\frac{dg^2(L)}{d \ln L} = (2-d)g^2 + 2(g^2)^2 \quad (112)$$

for the localization length did not have the factor $p_1^2 - \mathbf{p}_1 \cdot \mathbf{p}_2$. If this factor is included in the case of $0 < n < \frac{1}{2}$ and $d=1$, the bare conductance obtained from

Eqs. (66) and (91) gives a localization length which diverges like $\omega^{-(2n+1)}$ when Eq. (112) is used. This $\omega^{-(2n+1)}$ behavior is inconsistent with the result of Eq. (92), which is just the geometric mean of $\omega^{-1/(1-n)}$ of Eq. (93) and $\omega^{-(2n+1)}$. This suggests that, in the presence of long-range correlations, at least in $d=1$, the scaling relation of Eq. (112) is incompatible with Eq. (69) when the transport mean free path is used. The question is whether the single-parameter scaling relation of Eq. (112) should be modified if the transport relaxation time is relevant to the problem or the use of transport mean free path in the momentum cutoff of Eq. (69) is inadequate in the framework of VW. In fact, the use of transport mean free path for the momentum cutoff introduces additional length scale to the problem as can be seen from Eq. (69) where the quantity $\beta(E)$ of Eq. (68) is described by the single-phonon mean free path of Eq. (71). The presence of this new length scale, according to the theory of VW, has important consequences to the localization length. It changes the asymptotic behavior in $d=1$ and affects the prefactor in $d=2$. Since the mean free path and the localization length are the physical quantities which describe the transport properties of a system, we think that, in the case of long-range correlations, the transport relaxation time will play a certain role in determining the physical properties of the system. Further work is required to clarify this problem.

ACKNOWLEDGMENTS

The authors wish to thank Ping Sheng for useful discussions. The work was supported by the National Science Foundation of China.

APPENDIX

In the long-wavelength limit, V_p of Eq. (56) becomes $2Ka^2\mathbf{p}$, since $\gamma_p(E)$ in Eq. (63) has the asymptotic form $E^{2+\Delta}$ with $\Delta > 0$, as has been shown in Ref. 14 for all the correlation functions given in Eqs. (60) and (61). The function $\text{Im}R_p(E)$ in the integrand of Eqs. (53), (57), and (58) can be approximated by $-\pi \delta[\bar{m}(E^2 - \bar{c}^2 p^2)]$ and the momentum integrations become straightforward, leading to the Eqs. (65)–(67).

In order to derive Eq. (68) from Eq. (54) we use the results of Eqs. (58) and (65) and make the following approximations for Eq. (54):

$$\begin{aligned} \beta(E) &\cong \frac{-id\gamma^4 E^7}{4\pi\bar{m}\bar{c}^2\rho_{\text{ph}}(E)} \left(\frac{a}{2\pi} \right)^{2d} \int \int d\mathbf{p}_1 d\mathbf{p}_2 S(|\mathbf{p}_1 - \mathbf{p}_2|) S(|\mathbf{p}_1 + \mathbf{p}_2|) \Delta R_{p_1}^2(E) \Delta R_{p_2}(E) \\ &\cong \frac{-id\gamma^4 E^7}{4\pi\bar{m}\bar{c}^2\rho_{\text{ph}}(E)} \left(\frac{a}{2\pi} \right)^{2d} \int \int d\mathbf{p}_1 d\mathbf{p}_2 S(|\mathbf{p}_1 - \mathbf{p}_2|) S(|\mathbf{p}_1 + \mathbf{p}_2|) \Delta R_{p_1}(E) \Delta R_{p_2}(E) \frac{i}{\gamma_{p_1}(E)} \\ &\cong \frac{d\gamma^2 E^2}{8\pi\bar{m}\bar{c}^2\rho_{\text{ph}}(E)} \left(\frac{a}{2\pi} \right)^{2d} \int d\mathbf{p}_1 \Delta R_{p_1} \frac{\int d\Omega_{\hat{\mathbf{p}}} S(|\mathbf{p}_1 + \mathbf{p}|)}{\int d\Omega_{\hat{\mathbf{p}}}} \frac{1}{\gamma_{p_1}(E)} \int d\mathbf{p}_2 S(|\mathbf{p}_1 - \mathbf{p}_2|) \Delta R_{p_2}(E), \end{aligned}$$

where the peaked value of one of the $\Delta R_{p_1}(E)$ in the first integrand has been used to give the second integrand. By taking into account the fact that $\Delta R_{p_2}(E)$ has the peaked value when $p_2 = p = E/\bar{c}$ and the functions $S(|\mathbf{p}_1 - \mathbf{p}_2|)$ and $S(|\mathbf{p}_1 + \mathbf{p}_2|)$ cannot diverge simultaneously in the

case of long-range correlations, we have approximated the function $S(|\mathbf{p}_1 + \mathbf{p}_2|)$ by $\int d\Omega_{\hat{\mathbf{p}}} S(|\mathbf{p}_1 + \mathbf{p}|) / \int d\Omega_{\hat{\mathbf{p}}}$ in the last expression. Finally by using Eq. (63) twice, the last expression immediately gives Eq. (68).

-
- ¹See, for example, P. A. Lee and T. V. Ramakrishnan, *Rev. Mod. Phys.* **57**, 339 (1985).
- ²S. John, H. Sompolinsky, and M. J. Stephen, *Phys. Rev. B* **27**, 5592 (1983).
- ³S. John, *Phys. Rev. Lett.* **53**, 2169 (1984).
- ⁴P. W. Anderson, *Philos. Mag. B* **52**, 505 (1985).
- ⁵A. D. Zdetsis, C. M. Soukoulis, E. N. Economou, and G. S. Grest, *Phys. Rev. B* **32**, 7811 (1985).
- ⁶B. Bulka *et al.*, *Z. Phys. B* **60**, 13 (1985); **66**, 21 (1987).
- ⁷D. Vollhardt and P. Wolfe, *Phys. Rev. Lett.* **45**, 842 (1980); *Phys. Rev. B* **22**, 4666 (1980); *Phys. Rev. Lett.* **48**, 669 (1982).
- ⁸E. N. Economou, C. M. Soukoulis, and A. D. Zdetsis, *Phys. Rev. B* **30**, 1686 (1984).
- ⁹K. Arya, Z. B. Su, and J. L. Birman, *Phys. Rev. Lett.* **54**, 1559 (1985); **57**, 2725 (1986).
- ¹⁰T. R. Kirkpatrick, *Phys. Rev. B* **31**, 5746 (1985).
- ¹¹P. Sheng and Z. Q. Zhang, *Phys. Rev. Lett.* **57**, 1879 (1986).
- ¹²E. Akkermans and R. Marnard, *Phys. Rev. B* **32**, 7850 (1985).
- ¹³Q. J. Chu and Z. Q. Zhang, *Phys. Rev. B* **38**, 4906 (1988).
- ¹⁴S. John and M. J. Stephen, *Phys. Rev. B* **28**, 6358 (1983).
- ¹⁵J. Masek, *Z. Phys. B* **64**, 145 (1986).
- ¹⁶E. N. Economou, C. M. Soukoulis, and M. H. Cohen, *Phys. Rev. B* **37**, 4399 (1988).
- ¹⁷M. T. Beal-Monod and G. Forgacs, *Phys. Rev. B* **37**, 6646 (1988).
- ¹⁸Z. Q. Zhang and Q. J. Chu, *Phys. Lett. A* **131**, 507 (1988).
- ¹⁹E. A. Kotov and M. V. Sadovskii, *Z. Phys. B* **51**, 17 (1983).
- ²⁰M. H. Cohen, E. N. Economou, and C. M. Soukoulis, *Phys. Rev. B* **32**, 8268 (1985).
- ²¹E. N. Economou, *Green's Function In Quantum Physics*, 2nd ed. (Springer-Verlag, New York, 1983), Chap. 7.
- ²²E. N. Economou, C. M. Soukoulis, M. H. Cohen, and A. D. Zdetsis, *Phys. Rev. B* **31**, 6172 (1985).
- ²³E. Kolley and W. Kolley, *Z. Phys. B* **65**, 7 (1986).
- ²⁴Z. Q. Zhang and P. Sheng, *Phys. Rev. Lett.* **57**, 909 (1986).