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Localization and tunneling effects in percolating systems

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Localization and tunneling effects in percolating systems are studied using the homomorphic-cluster and coherent-potential approximations. The localization behavior of the electron states and hence the mobility edges are analyzed by means of the localization functions $L(E)$ and $F(E)$. When tunneling is neglected, the problem at hand reduces to the ordinary quantum percolation model. As the tunneling strength is increased, the percolation threshold decreases and no localization transition occurs when the tunneling is sufficiently strong.

I. INTRODUCTION

There has been considerable interest in recent years in studying localization effects in percolating systems.[1–8] In the classical percolation picture, we are concerned only with geometrical connection. Sites or bonds in a lattice are blocked or broken at random, and the question to be asked is if there exists an infinite percolative channel of unblocked sites or unbroken bonds. This underlying geometrical structure reveals various physical properties of disordered materials. If a percolative channel exists, a classical particle or fluid can diffuse infinitely far from its initial position. This may not be the case for a quantum particle.

Quantum effects in percolation processes have been studied on the basis of a tight-binding Hamiltonian where the sites are randomly assigned with zero or infinite site energy (site model), or the bonds are assigned with zero or unit transfer energy (bond model).[9] The infinite site energy in the site problem or the zero transfer energy in the bond problem acts as a blockage for propagation of a quantum particle. The microscopic disorder in the structure gives rise to scattering of the particle which in turn causes quantum localization of the particle and affects the percolation transition. Since quantum particles cannot propagate before the classical percolation threshold is reached, the quantum threshold must be larger than or equal to the classical one. There have been many estimations of percolation threshold for the quantum percolation model. Results for two dimensions are ambiguous but believed to be unity or close to unity.[4,10] For the simple-cubic lattice, most estimations centered around 0.35 for the bond problem[4,10] and 0.45 for the site problem.[11] Instead of the discrete models described above, one can also study continuum models from a dynamical point of view.[12]

The infinite site energy or the zero transfer energy in the quantum percolation problems is to simulate the existence of a potential barrier which prohibits the propagation of a quantum particle and makes the quantum problem formally similar to the classical problem. In real systems, however, the potential barrier may not be literally infinite even though it prohibits propagation of a classical particle and the classical percolation picture is still valid for classical particles. For quantum particles, the finiteness of the potential barrier height brings in another important quantum effect, namely, tunneling effect which has been ignored in the previous studies of quantum percolation. The purpose of the present paper is to investigate quantum tunneling effects on percolation process.

It is physically interesting and important to study quantum tunneling effects since they realistically reflect the physical situation of disordered materials. Quantum tunneling can be incorporated in the quantum percolation model by reducing the barrier height of the infinite potential, which makes blocks in the quantum percolation model, to a finite value so that the tunneling probability is nonzero. When tunneling is taken into consideration, it competes with the localization effect and tends to reduce the percolation threshold. We study in this paper how quantum tunneling affects the percolation threshold and the mobility edge.

We consider a system described by a tight-binding Hamiltonian:

$$H=\sum_{n}\varepsilon_n\,|\,n\,\rangle\langle\,n\,|+\sum_{\substack{n,m\\ n\neq m}}|\,n\,\rangle t_{nm}\langle\,m\,|\ , \tag{1.1}$$

where $|\,n\,\rangle$ is the Wannier function associated with an atom located at site n, and the transfer energy t_{nm} is nonzero only if n and m are nearest neighbors.

For the site percolation model with tunneling, the tight-binding Hamiltonian (1.1) is subject to the following probability distribution for the site energy ε_n:

$$P(\varepsilon_n)=x\delta(\varepsilon_n)+(1-x)\delta(\varepsilon_n-\varepsilon)\ ,\qquad 1\geq x\geq 0,\quad \infty\geq\varepsilon\geq 0\ , \tag{1.2}$$

and the transfer energy t_{nm} is set to unity. Similarly, for the bond percolation model, the site energy ε_n is set to zero and the transfer energy t_{nm} obeys the probability distribution

$$P(t_{nm})=p\delta(t_{nm}-1)+(1-p)\delta(t_{nm}-t)\ ,\qquad 1\geq p\geq 0,\quad 1\geq t\geq 0\ . \tag{1.3}$$

Nonvanishing t (or finite ε) represents a finite probability of tunneling through the barrier. The cases where $\varepsilon=\infty$ and $t=0$ correspond to the ordinary quantum percolation limit.[9,13,14]

At this juncture, it may be appropriate to distinguish our present problem from that of the Anderson localization[15] problem even though there is a transition of Anderson type in our problem. The Anderson model is essentially a tight-binding model of a lattice with the disorder introduced by assuming randomly distributed site energy. The site disorder variable in the Anderson model is drawn from a continuous probability distribution, typically a uniform one and the transition is governed by the ratio of the width of the distribution and the transfer energy. In our case, the width of distribution as determined by the second moment is $x(1-x)\varepsilon^2$ for the site model and the distribution is therefore most random at $x=0.5$. For systems with off-diagonal disorder, it has been suggested that the distribution of $\log|t|$ is a relevant measure for off-diagonal randomness.[16–18] The second moment of the distribution Eq. (1.3) for the bond problem is $p(1-p)(\log_{10}|t|)^2$ which is the largest at $p=0.5$. As we shall see later, localization transition does not necessarily occur at this concentration. Furthermore, in the ordinary quantum percolation limit, the width of distribution tends to infinity in any dimensions and according to the conventional argument all states are supposed to be localized. However, it is generally believed that there exists a critical value of the parameter x or p at which a localization transition takes place except for one and two dimensions where arbitrary randomness causes states to localize.[19] It is thus clear that the distribution involved in quantum percolation process should be considered as a class different from the standard Anderson model.

The coherent-potential approximation[20] (CPA) and the homomorphic-cluster coherent-potential approximation[21,22] (HCPA) are used to obtain the average Green's functions for the site and bond problem, respectively. The effective medium to be determined self-consistently is assumed to be a lattice having a semielliptic unperturbed density of states in three dimensions. The $L(E)$ (Refs. 23 and 24) criterion is used to study the mobility edges for the site problem. A modified criterion $F^*(E)$ is proposed for the bond problem.

We will see that the percolation threshold is a decreasing function of the tunneling strength and disappears at certain tunneling strength.

In Sec. II of this paper, basic formalism of CPA and HCPA is presented. Section III is devoted to a presentation of results for the bond and site problems. The final section contains a discussion.

II. BASIC FORMALISM OF HOMOMORPHIC-CLUSTER AND COHERENT-POTENTIAL APPROXIMATION

Consider a sample of diagonally disordered system described by Hamiltonian (1.1). We may set $t_{nm}=t$, some constant transfer energy. We approximate the tight-binding Hamiltonian (1.1) by

$$H_A=H_c+|1\rangle(\varepsilon_1-\sigma)\langle 1|\equiv H_c+V\ , \tag{2.1}$$

where

$$H_c=\sum_n |n\rangle\sigma\langle n|+\sum_{\substack{n,m\\ n\neq m}} t\,|n\rangle\langle m| \tag{2.2}$$

is called the coherent Hamiltonian. Physically speaking, this means that the system behaves as if a coherent potential σ has been assigned to each lattice site except site 1 which has the random potential ε_1. V can be treated as a perturbation of the uniform medium and the scattering t matrix is

$$T=V(1-G^cV)^{-1}\ , \tag{2.3}$$

where G^c is the propagator for the uniform coherent medium.

The coherent potential approximation says that the Green's function for the coherent medium is equal to the ensemble average of the Green's function for the approximate Hamiltonian, that is

$$\frac{1}{z-H_c}=\left\langle\frac{1}{z-H_A}\right\rangle\ , \tag{2.4}$$

which turns out to be equivalent to $\langle T\rangle=0$. $\langle\cdots\rangle$ denotes ensemble average over ε_1. Note that, due to the form of the perturbing potential, all matrix elements of T except the (1,1) element are identically zero. Written out in full, the CPA condition is

$$\left\langle\frac{\varepsilon_1-\sigma}{1-G_{11}^c(\varepsilon_1-\sigma)}\right\rangle=0\ , \tag{2.5}$$

where G_{11}^c is the diagonal element of the coherent-medium propagator, and is given by

$$G_{11}^c(z)=\int\frac{\rho_0(E)}{z-\sigma-E}dE\ . \tag{2.6}$$

$\rho_0(E)$ is the density of states for the regular system H_c with $\sigma=0$. The off-diagonal element of the coherent medium propagator is given by

$$G_{12}^c(z)=\frac{(z-\sigma)G_{11}^c-1}{nt}\ , \tag{2.7}$$

where n is the coordination number.

The above formalism works well for the average one-particle Green's function in disordered systems with diagonal disorder. For systems with purely off-diagonal disorder, the homomorphic-cluster coherent-potential approximation (HCPA) is used. We can set $\varepsilon_n=0$ in Eq. (1.1) so that the Hamiltonian for the system is

$$H=\sum_{\substack{n,m\\ n\neq m}}|n\rangle t_{nm}\langle m|\ . \tag{2.8}$$

The whole system except for a neighboring pair of sites denoted by 1 and 2, is replaced by an effective medium defined by

$$H_{\rm eff}=\sum_n |n\rangle\sigma_d\langle n|+\sum_{\substack{n,m\\ n\neq m}}|n\rangle\sigma_{od}\langle m|\ . \tag{2.9}$$

The Hamiltonian (2.8) is approximated by

$$H_A=H_{\rm eff}+V\ , \tag{2.10}$$

where

$$V=|c\}\{c|(H-H_{\rm eff})|c\}\{c| \tag{2.11}$$

and

$$|c\}=(|1\rangle,|2\rangle)\ . \tag{2.12}$$

To ensure analyticity of the approximation,[21] we partition both sites 1 and 2 into n subunits, one of which is considered to belong to the pair and others to the effective medium. The self-consistent condition now reads as a 2×2 matrix equation

$$\langle \tilde{V}(\tilde{1}-\tilde{G}\tilde{V})^{-1}\rangle = 0 \tag{2.13}$$

in which

$$\tilde{G}=\begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix}$$

and

$$\tilde{V}=\begin{bmatrix} -\frac{1}{n}\sigma_d & t_{12}-\sigma_{od} \\ t_{21}-\sigma_{od} & -\frac{1}{n}\sigma_d \end{bmatrix} . \tag{2.14}$$

Analogous to the single-site CPA, the matrix elements of $\tilde{G}$ are given as

$$G_{11}(z)=\int \frac{\rho_0(E)}{z-\sigma_d-(\sigma_{od}/t)E}dE \tag{2.15}$$

and

$$G_{12}(z)=\frac{1}{n\sigma_{od}}[(z-\sigma_d)G_{11}-1] \tag{2.16}$$

with $\rho_0(E)$ denoting the density of states for a regular lattice of the same structure as the effective medium with site energy 0 and nearest neighbor transfer energy t.

For the pairwise cluster under consideration, it is clear that $t_{12}=t_{21}$ and $G_{11}=G_{22}$, $G_{12}=G_{21}$. We can then easily diagonalize the matrices $\tilde{G}$ and $\tilde{V}$ by a similarity transformation, and the self-consistent condition reads

$$\left\langle \frac{-\frac{1}{n}\sigma_d \pm \sigma_{od} \mp t_{12}}{1-(G_{11}\mp G_{12})\left[-\frac{1}{n}\sigma_d \pm \sigma_{od} \mp t_{12}\right]} \right\rangle = 0 . \tag{2.17}$$

$\langle \cdots \rangle$ denotes average over the distribution of t_{12}.

III. RESULTS

In this section, we shall discuss the results of numerical calculation for a three-dimensional system. The unperturbed density of states will be approximated by a semielliptic Hubbard band in order to avoid the complication of the numerical work involved in an exact treatment of a simple-cubic band. To make the system reflect its three-dimensional aspect, we shall take $n=6$ which corresponds to the number of nearest neighbors in a simple cubic lattice.

A. Bond problem

The diagonal Green's function for the Hubbard band satisfies

$$\frac{B^2G_{11}^2}{4}-(z-\sigma_d)G_{11}+1=0 , \tag{3.1}$$

where $B=n\sigma_{od}$, and from Eq. (2.16), the off-diagonal Green's function is

$$G_{12}=\frac{n\sigma_{od}}{4}G_{11}^2 . \tag{3.2}$$

With the probability distribution Eq. (1.3), the self-consistent condition Eq. (2.17) becomes

$$\frac{p}{1+G_\pm(\sigma_\pm-1)}+\frac{1-p}{1+G_\pm(\sigma_\pm-t)}=1 , \tag{3.3}$$

where

$$G_\pm=G_{12}\pm G_{11}$$

and

$$\sigma_\pm=\sigma_{od}\pm\frac{1}{n}\sigma_d .$$

The density of states is given by

$$\rho(E)=-\frac{1}{\pi}\text{Im}\,G_{11} . \tag{3.4}$$

Figure 1 shows the density of states as a function of the energy E and the concentration p when $t=0.1$ [Fig. 1(a)] and 0.01 [Fig. 1(b)]. Note that spectral gaps appear near $E=\pm 1$ when $p\approx 0$. This can be seen more clearly in Fig. 2 in which the band edges are shown. In fact, the impurity levels at $p=0$ due to a single impurity bond of strength

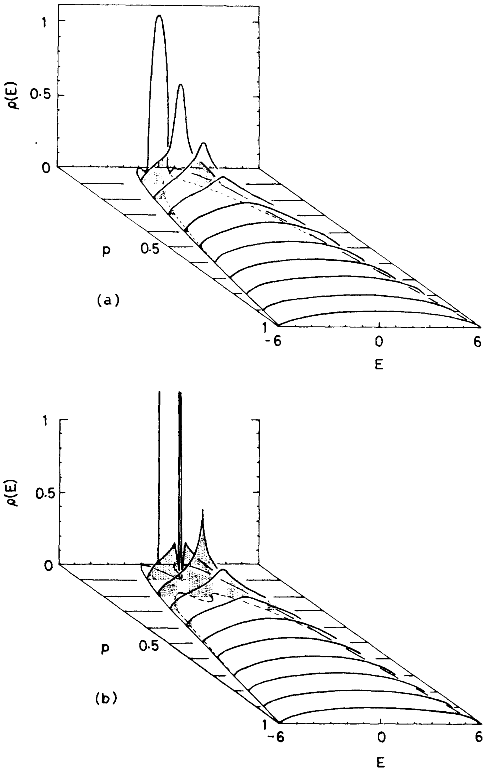

FIG. 1. Density of states for the quantum bond percolation model with tunneling. States in the shaded part are localized. The dashed lines are the mobility edges. (a) $t=0.1$, (b) $t=0.01$.

t appears at

$$E_{\pm}=\pm\frac{(\delta-b)}{2}\pm\frac{1}{2\delta}\sqrt{\delta^2(\delta-b)^2+\delta b(b^2+2b\delta+5\delta^2)}\ , \tag{3.5}$$

where $\delta=t-t_1$ and $b=6t_1$, t_1 being the background bond strength and is equal to unity in our case.

To locate the mobility edges, we employ a criterion which is modified from $F(E)$ function introduced for systems with only diagonal disorder prevails[23]

$$F^*(E)=\left|\frac{6\sigma_{od}}{E-\sigma_d}\right| . \tag{3.6}$$

The trajectory $F^*(E)=1$ separates the energy spectrum into regions of localized (<1) and extended (>1) states. Those states in the shaded area of the density of states in Fig. 1 are localized, and the mobility edges are shown with dashed lines.

When the tunneling strength t is reduced, the mobility edges move inward and eventually merge at $t\approx 0.03$ [Fig. 2(b)]. For $t<0.03$, all states become localized for a limited range of p [Figs. 2(c) and 2(d)] which is far from the range at which the variance of the distribution is largest. It is, therefore, natural to regard the concentration at which the state at $E=0$ becomes localized when p is reduced for a given t as the percolation threshold for the quantum percolation problem with tunneling. Thus the percolation threshold p_c exists only for $t \lesssim 0.03$. In Fig. 3, the percolation threshold p_c is plotted against $-\log|t|$. The extrapolation of p_c to $t=0$ corresponds to the quantum percolation threshold for processes without tunneling. This limiting value $p^*=0.252$ is larger than the classical one but smaller than other estimates of the quantum percolation threshold.[4,10]

B. Site problem

For the case of a system with diagonal disorder, the Hamiltonian treated is

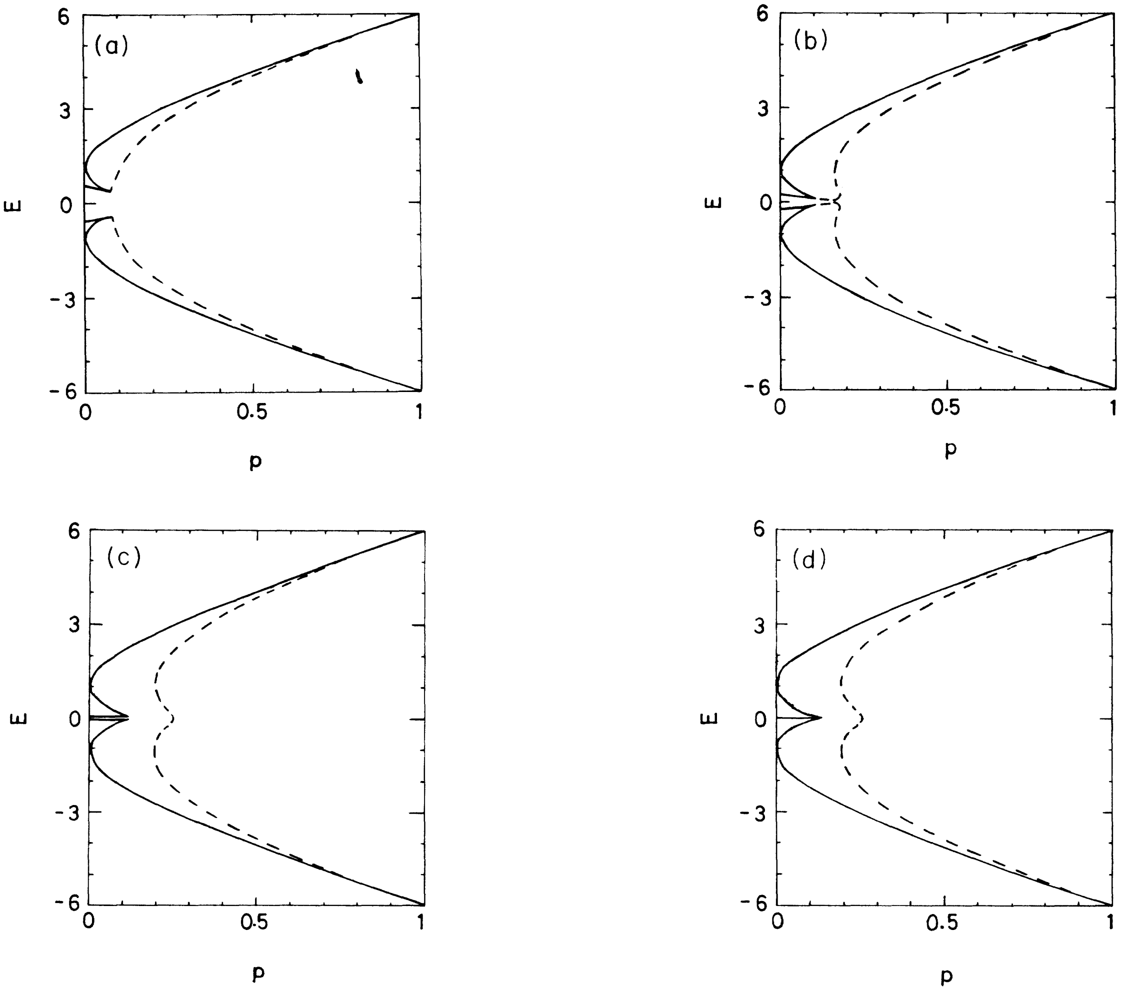

FIG. 2. Band edges (solid curve) and mobility edges (dashed curve) for the quantum bond percolation model with tunneling. (a) $t=0.1$, (b) $t=0.03$, (c) $t=0.01$, (d) $t=10^{-6}$.

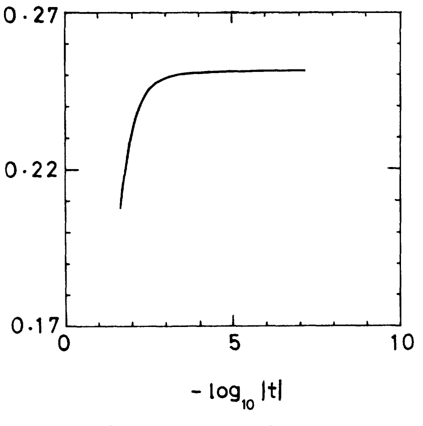

FIG. 3. Critical concentration p_c vs $-\log_{10}|t|$.

$$H=\sum_n \varepsilon_n |n\rangle\langle n| + \sum_{\substack{n,m\\ n\neq m}} |n\rangle\langle n| \ , \qquad (3.7)$$

where ε_n has the probability distribution given in Eq. (1.2).

The self-consistent equation (2.5) with distribution (1.2) is reducible to a third-order polynomial equation for the diagonal element of the Green's function:

$$81\,G_{11}^3+9(\varepsilon-2E)G_{11}^2 +[E(E-\varepsilon)+9]G_{11}+(x\varepsilon-E)=0 \ . \qquad (3.8)$$

We employ a localization function:

$$L(E)=K\left|G_{11}-\frac{G_{12}G_{21}}{G_{11}}\right| \ , \qquad (3.9)$$

where $K=4.6826$ is the connectivity constant for the simple cubic lattice.[24]

The parameter ε measures the tunneling strength. The limit where ε goes to infinity corresponds to the usual quantum percolation since the infinite potential barrier forbids tunneling. In Fig. 4, the band edges and mobility edges are shown. The energy band splits into two when $\varepsilon=6.0$. Only the lower band is shown in Fig. 4(c). No substantial changes are observed in these diagrams for $\varepsilon>100$.

We are primarily interested in the lower band associated with levels at $E=0$. When p is reduced from unity, localized states first appear near the band edges and eventually coalesce near the band center. The corresponding value of x is considered to be the percolation threshold for the particular tunneling strength. When $\varepsilon<5.166$, the threshold cannot be defined.

In Fig. 5, the percolation threshold x_c is plotted against $1/\varepsilon$. The limiting value of $x_c\sim 0.26$ at $\varepsilon=\infty$ is the quantum percolation threshold for processes without tunneling.

IV. DISCUSSION

We have studied the quantum percolation model with tunneling. The homomorphic-cluster CPA and CPA are used to study the bond and site problems, respectively. A major difference of the present work from others is the inclusion of tunneling effects. Tunneling is incorporated in the site problem by considering a finite potential barrier on a blocked site instead of an infinite one. Similarly, nonvanishing transfer energy between a pair of sites whose bond is broken is the corresponding tunneling effect in the bond problem. When tunneling is included, it competes with the localization effect and enhances the

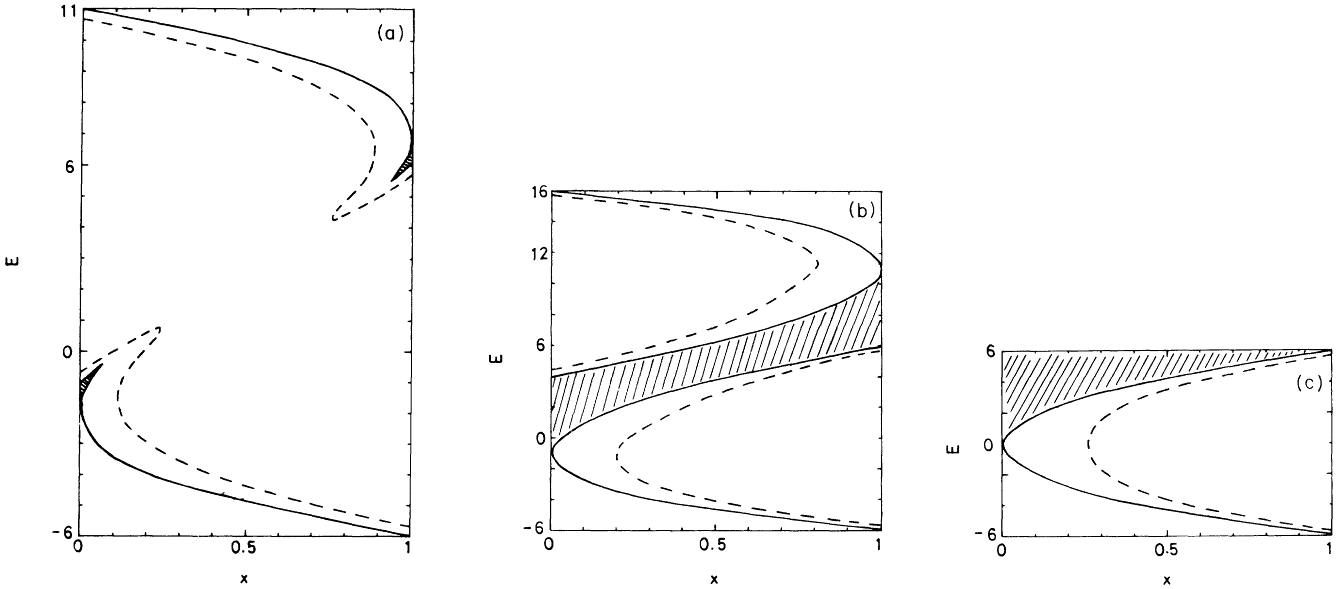

FIG. 4. Band edges (solid curve) and mobility edges (dashed curve) for the quantum site percolation model with tunneling. The shaded regions are band gaps. The mobility edges are obtained using $L(E)$ criterion. (a) $\varepsilon=5$, (b) $\varepsilon=10$, (c) $\varepsilon=100$ (only the lower band is shown).

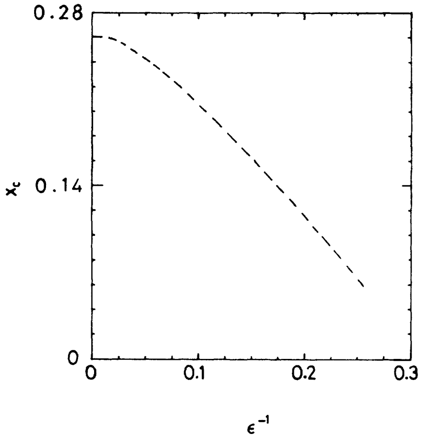

FIG. 5. Critical concentration x_c vs $1/\varepsilon$.

percolation probability. In fact, our result demonstrates that the percolation threshold is a decreasing function of the tunneling strength and disappears when the tunneling is sufficiently strong.

Tunneling effects are important and interesting because they greatly enhance the applicability of the percolation theory. In the classical percolation picture, there are only two phases, namely, percolated or nonpercolated, since we are only concerned with geometrical connection. The scenario is enriched when quantum percolation is considered. The present consensus that the classical and quantum percolation thresholds are significantly different immediately implies the existence of three phases: classically localized, quantum localized, and extended. When tunneling is neglected, the above three phases appear in that order when the fraction of broken bonds or infinite barriers is reduced. If the tunneling is sufficiently weak, we would expect to have similar phases. As the tunneling strength increases, the quantum percolation threshold decreases and will eventually cross over the classical percolation threshold. In this case, the quantum percolation threshold is smaller than its classical counterpart and now the three phases are localized, quantum tunneling, and extended. Localization transition does not take place when tunneling is sufficiently strong ($t > 0.03$ for bond problem and $\varepsilon < 5.166$ for site problem in the present approximation). Certain experiments[3,25] that show more than two phases near the classical percolation threshold may be explained in terms of the quantum percolation.

We can extrapolate our results to the limiting situation where tunneling is neglected. Such limit is the ordinary quantum percolation. Although the thresholds obtained by extrapolation are somewhat smaller than those reported in previous works, and in the case of the site problem it is smaller than its classical counterpart, our result clearly illustrates the qualitative behavior of electron localization and the mobility edges correctly when tunneling effects are included in the quantum percolation process.

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