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Localization in two-dimensional quantum percolation

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The quantum site and bond percolation problem, which is defined by a disordered tight-binding Hamiltonian with a binary probability distribution, is studied using finite-size-scaling methods. For the simple square lattice, we find that all states are exponentially localized for any amount of disorder, in agreement with the scaling theory of localization and in disagreement with recent claims of a localization transition in two dimensions. The localization length λ is given by $A\exp\{B[p/(1-p)]^y\}$ with y very close to 0.5 and p the probability that a site or a bond is present.

Considerable progress has been made in our understanding of the effects of disorder[1-8] on the nature of the electronic wave function. It is now well established that for dimensions $d \geq 3$, there is a localization transition between extended and localized states, as the strength of the disorder increases. Complete localization is predicted for $d \leq 2$ by the one-parameter scaling theory.[2,3] This scaling theory is supported by a large number of numerical studies in $d=2$ and 3.[5-8] According to the scaling theory, there are no extended states in $d=2$ for any amount of disorder, no matter how weak. Instead, all states should be exponentially localized with a localization length λ that has the form $\lambda \sim \exp(W^{-2})$, where W is strength of the disorder. Since it is possible to have extremely large localization lengths for small W, the establishment of exponential localization in $d=2$ for weak disorder by numerical techniques is difficult.[5-9] A few recent studies have questioned the one-parameter scaling theory and even suggested that there exists a transition to extended states at finite disorder in $d=2$. Most of these studies have been for the case of bond[10] or site[11] quantum percolation. If this result was true, then the single scaling theory of localization would have to be modified as has been suggested in some recent theoretical studies.[12]

The purpose of the present paper is to present a detailed numerical study of the quantum site and bond percolation problem in $d=2$ using the very reliable transfer-matrix technique and finite-size scaling.[5-8] The present results which are for very large lattice sizes give very strong and we believe convincing evidence that no localization transition occurs for any amount of disorder in $d=2$. Traces of a transition at finite disorder in $d=2$, seen in these two studies,[10,11] are due to the rich structure of the density of states (DOS) in the site as well as the bond quantum percolation models.

Quantum percolation is usually formulated in terms of a tight-binding one-electron Hamiltonian on a regular lattice

$$H=\sum_n |n\rangle \varepsilon_n \langle n| + \sum_{\substack{n,m \\ (n\neq m)}} |n\rangle V_{nm} \langle m| , \qquad (1)$$

where the transfer energy V_{nm} vanishes, unless n and m are nearest neighbors and $|n\rangle$ represents a wave function localized near site n. As in the classical case, we can define site and bond quantum percolation. In the site percolation problem, the site energy ε_n is assumed to obey the distribution

$$P(\varepsilon_n)=p\delta(\varepsilon_n-\varepsilon_A)+(1-p)\delta(\varepsilon_n-\varepsilon_B),\ \varepsilon_B=-\varepsilon_A \qquad (2)$$

where $\delta=|\varepsilon_A-\varepsilon_B|/zV=2\varepsilon_A/zV$ determines the degree of disorder, z is the number of nearest neighbors, and $V_{nm}=V$ is a constant. In the bond percolation, the site energies ε_n are constant, and may be arbitrarily taken to be zero, $\varepsilon_n=0$, while the nearest-neighbor transfer energies V_{nm} distributed according to

$$P(V_{nm})=p\delta(V_{nm}-V)+(1-p)\delta(V_{nm}-V_B) \qquad (3)$$

with $V_B=0$. These probability distributions are essentially characterized by two parameters: p, the concentration of A atoms (bonds), i.e., the probability that a given site (bond) is occupied, and $\varepsilon_A(V)$. One important limiting case is that of the binary-alloy distribution when $\varepsilon_A \to \infty$ ($V_B \to 0$). In this case, the only way an electron being initially at an A (B) site or a V bond may propagate across the sample is to find a path consisting entirely of A (B) sites or V bonds which percolates. Percolation theory examines exactly this problem, i.e., the probability of finding such an exclusive A path or V bond. Therefore, sites with infinite site energy and bonds with zero transfer energy represent blocks for the motion of a quantum particle governed by the Schrödinger equation with the Hamiltonian in Eq. (1).

The main concern in quantum percolation problems is to locate the quantum percolation threshold p_q for the site and the bond case, below which all eigenstates of the Hamiltonian are localized. It is clear that the quantum threshold must be greater than its classical counterpart p_c, since the existence of an infinite cluster is a necessary but not sufficient condition for the existence of an extended state.

There have been a number of estimations[11,13-17] of the quantum percolation threshold for the site and the bond cases, both for the square and simple cubic lattices. While all the different numerical methods clearly show that p_q is

greater than p_c, there is no agreement on its precise numerical value for the site as well as the bond case both in the square and cubic lattices. Numerical estimates[11,13–17] of quantum site percolation thresholds range from 0.59 to above 0.94 for the square and from 0.38 to 0.48 for the simple cubic lattice. The most recent calculations[11,13–15] with large size systems using the scaling hypothesis or related approaches, narrow the range of p_q to $0.42 \leq p_q \leq 0.48$, with $p_q = 0.44$ as the best estimate for the quantum site percolation threshold of the simple cubic lattice. For quantum bond percolation, the thresholds range from 0.50 to above 0.94 for the square lattice and from 0.30 to 0.55 for the simple cubic lattice. More recent[10,15,17] calculations narrow this range to $0.30 \leq p_q \leq 0.39$, with $p_q = 0.32$ being the best estimate for the quantum bond percolation threshold on the simple cubic lattice. The classical site (bond) percolations thresholds[18] are 0.59 (0.50) for the square lattice and 0.31 (0.25) for the simple cubic lattice, respectively.

In this present paper we concentrate on $d=2$, since there are two recent numerical calculations[10,11] that suggest a localization transition for $p_q < 1$ in contradiction to the scaling theory of localization. Meir, Aharony, and Harris[10] carried out a series analysis of the average transmission coefficient for the quantum bond percolation model which reproduces quite well all known results for $d \geq 3$. They argue, however, that their series expansion strongly suggests the existence of a localization transition with p_q in the range 0.6–0.8 in $d=2$. This result is in disagreement with their own earlier series[19] analysis of the inverse participation ratio which gave $p_q = 1.0$ and with the one-parameter scaling theory. It is, therefore, very important to resolve the issue of the existence or nonexistence of a localization transition in $d=2$, for both the site and bond quantum percolation problems. We believe this can be done only by using a very accurate numerical approach. To date, finite-size-scaling analysis using the transfer-matrix technique has proven to be the most reliable technique for problems of this type[5–8] and we apply it here to these two cases.

In the transfer-matrix method, one considers coupled $d=1$ systems. Each $d=1$ system is described by a tight-binding Hamiltonian of the form given by Eq. (1). In our explicit results for this study, we assume that the probability distribution $p(\varepsilon_n)$ of the random sites and $p(V_{nm})$ of the random bonds are described by Eqs. (2) and (3), respectively. [In previous numerical calculations,[8] we have systematically studied the behavior of the tight-binding disordered systems when $p(\varepsilon_n)$ is given by either a rectangular or a Gaussian probability distribution.] The corresponding sites or bonds of the nearest-neighbor $d=1$ system are coupled together by an interchain matrix element. In two dimensions, we study systems of width M and length N, while in $d=3$ the systems have a square cross sectional area of M^2. We use periodic boundary conditions in the direction(s) perpendicular to the axis of the $d=1$ chains. Using the transfer-matrix technique,[5–8] we determine numerically the largest localization length λ_M for each value of the width M. From a plot of λ_M vs M, one can determine the localization properties of the system. One finds two distinct behaviors of the function λ_M vs M. In the first case, which corresponds to a localized state, the second derivative $d^2\lambda_M/dM^2$ is negative and λ_M approaches a finite value λ as $M \to \infty$, where λ is the localization length of the resulting $d=2$ ($d=3$) disordered system. In the second case, which corresponds to an extended state, $d^2\lambda_M/dM^2$ is positive and $\lambda_M \to \infty$ as $M \to \infty$. At exactly the mobility edge, we have found for a number of disordered tight-binding models[8,13] in $d=3$ with a rectangular, Gaussian, or binary probability for the site energies that $\lambda_M/M \simeq 0.6$.

We calculated λ_M on the square lattice for $0.5 \leq p \leq 0.85$, and $M = 8$, 16, 32, 64, and 128. The length N of the M coupled chains was at least 20000. For the site problem, we choose $\varepsilon_A = 50.00$, i.e., $\delta = 2\varepsilon_A/zV = 25$ and the energy E is measured from the center of the A subband, i.e., $E=0$, corresponds to $E=\varepsilon_A$ in Eq. (2). We calculated λ_M for $E = 0.05$, 0.25, 1.05, and -0.05. For the bond problem, we used the probability distribution given by Eq. (3) with $V=1$, V_B was taken to be a very small number. Our results were independent of the value of V_B, provided $V_B \leq 10^{-4}$. We used a nonzero value of V_B, since for finite M there is always a finite probability that the system would break into several disconnected pieces. We also calculated λ_M for $E = 0.05$, 0.25, and

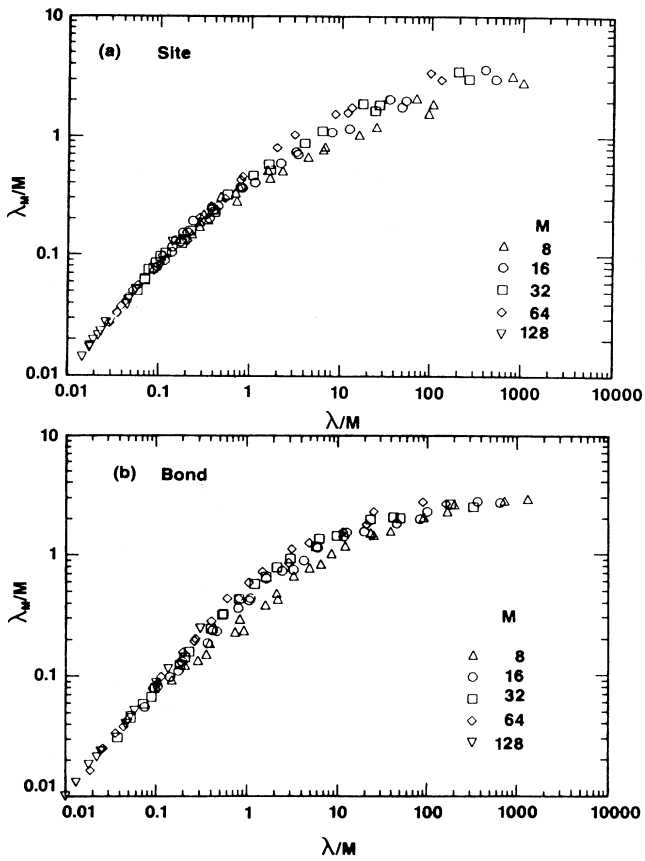

FIG. 1. Localization length λ_M/M vs λ/M for various values of the concentration p and several values of the energy E for the (a) site and (b) bond quantum percolation model on the square lattice. There is only one branch in the universal curve, so that all the states are exponentially localized.

1.05. In agreement with previous numerical results[5-8] for the ordinary Anderson localization problem, we find that all of our results for λ_M for different energies E and probabilities p both for the site and bond quantum percolation model tend to follow the one-parameter scaling curve. In Fig. 1, we plot λ_M/M vs λ/M for all the different cases considered, corresponding to the various energies, probabilities p, and widths M. Notice that all the points are clustered around a universal curve. There is considerable dispersion due to numerical errors, which are appreciable since we are dealing with rather large λ or λ_M in most of the cases. As a result of these uncertainties, we estimate that our numerical results for λ, plotted in Fig. 2, are accurate to no more than 10%–20% for large localization lengths. When λ is small, the relative error is much lower, i.e., about 2%. This uncertainty could be reduced somehow at the expense of increasing substantially the computer time. (An error of about 2% in λ_M requires the length N to be about 10^4 times the localization length λ_M.) We have plotted the results for λ in Fig. 2 this particular way to point out the fact that the localization length appears to have the form

$$\lambda = A\exp\{B[p/(1-p)]^{1/2}\}, \tag{4}$$

where the constants A and B depend on the energy E. For the site case, we find that the pair $(A,B)=(0.004,6.00)$, $(0.0035,6.20)$, and $(0.005,6.00)$ for $E=0.25$, 1.25, and -0.05. For the bond case, we have that $(A,B)=(0.0045,5.35)$, $(0.015,5.45)$, and $(0.015,5.70)$ for $E=0.05$, 0.25, and 1.05. Notice that the dependence of λ on p is very strong and that λ becomes extremely large as $p\to 1$. It is only with the finite-size-scaling method that one can make some statements about the localization properties of the site or the bond quantum percolation problem in the weak disorder limit, $p\to 1$. Our numerical results clearly show that the scaling theory of localization is well obeyed in $d=2$ for the site and the bond quantum percolation problem. All the states are exponentially localized and the localization length λ has the exponential dependence given by Eq. (4), which shows that λ is extremely large as $p\to 1$. This is reminiscent[8] of the $d=2$ case of the Anderson localization problem with a rectangular probability distribution of the site energies ε_n. Loring and Mukamel[20] have also calculated the localization length λ for $d=2$ in the site quantum percolation problem with a self-consistent mode-coupling theory. They find that λ has the form $A\exp[Bp/(1-p)]$. Our numerical results suggest that the form given by Eq. (4) fits the data better than that of Loring and Mukamel.[20] We do not understand this difference. However, the difference is probably not of great significance, since both forms give exponentially large localization lengths as $p\to 1$. In Fig. 2(a), we also show λ for $E=0.05$ for the site case. In this case, we know that the DOS has a very fine structure[13,21] in both the site[21] and bond case.[17] For site quantum percolation on the square lattice, there is a gap in the DOS around $E=-0.05$ for small values of p. As p increases, the gap decreases and finally closes for $p>0.70$. The structure in the DOS is also reflected in the localization length calculated by the transfer-matrix method. λ is very small when there is a gap in the DOS

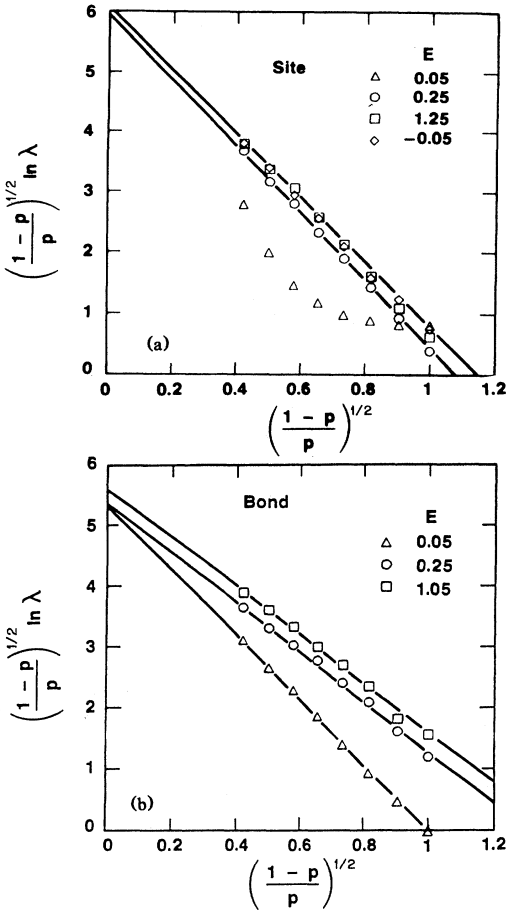

FIG. 2. $[(1-p)/p]^{1/2}\ln\lambda$ vs $[(1-p)/p]^{1/2}$ for the (a) site and (b) bond quantum percolation model on a square lattice for different values of the energy E. The localization length λ is given by $A\exp[B(p/1-p)^{1/2}]$ in agreement with the scaling theory of localization.

and starts to increase only when $p\gtrsim 0.7$. We believe this is why Meir, Aharony, and Harris[10] found a localization transition for $p\simeq 0.6$–0.8 for $E=0.05$, from their series expansion for the transmission coefficient in $d=2$ for the bond case. This problem did not arise in the series expansion[19] of the inverse participation ratio, since there they averaged over a width of energies, not just one. This averaging smears out the structure in the DOS and therefore gives a more accurate estimate for the localization length. These gaps in the density of states also occur in higher dimension, although at different energies than in two dimensions, and the widths of the gaps are narrower.

In conclusion, we have calculated, using the very accurate method of the finite-size scaling, the quantum percolation threshold for site and bond in the square lattice. We find that all the states are exponential localized in agreement with the scaling theory of localization. The localization length λ is found to behave approximately as $A\exp\{A[p/(1-p)]^{1/2}\}$. The previous discrepancies concerning the quantum percolation thresholds in $d=2$ are partially due to the rich structure of the DOS and partially to the extremely large values of λ as $p\to 1$.

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