Mobility edges for the quantum percolation problem in two and three dimensions

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Numerical results are reported for the quantum site-percolation problem. For the square lattice and the simple cubic lattice quantum percolation thresholds p_q are calculated by studying the sensitivity of eigenvalues to a change in boundary conditions. Observing the energy dependence of the transition from localized to extended states, mobility edge trajectories are calculated. We obtain $p_q=0.45$ in three dimensions and $p_q=0.70$ in two dimensions. The latter value of p_q is identified with a transition from weakly to strongly localized states, according to a similar localization behavior observed for the Anderson problem.

I. INTRODUCTION

Condensed systems with a large degree of disorder are abundant in nature and frequently have remarkable properties. Theoretically such systems cannot be treated as regular systems with a small perturbation. Thus their characterization poses a substantial problem. One of the attempts to characterize disordered systems is by the localized or extended nature of their eigenfunctions of a quantum-mechanical Hamiltonian. This character necessarily has a strong effect on transport properties. In the present article we shall deal with these properties of localization.

In a disordered system, all eigenfunctions become localized when the strength of disorder exceeds some specific value. This fundamental theorem is due to Anderson's study of a tight-binding Hamiltonian.[1] The operator of the Anderson Hamiltonian reads

$$\hat{H}|i\rangle=\varepsilon_i|i\rangle+\sum_{j\neq i}V_{ij}|j\rangle\ . \tag{1}$$

$\hat{H}$ acts on an atomic orbital located at site i. This sum has to be taken over all nearest neighbors of i. All atomic orbitals are assumed to be orthogonal. In the original model, the interactions between different sites are kept constant and only the diagonal elements of the Hamiltonian vary within a uniform distribution of width W. If W/V exceeds W_c/V, all states become localized, so there is no carrier transport at zero-degree temperature. For a given $W<W_c$, the spectrum can be divided into a part where all states are localized and another part where in addition to the localized states extended ones occur. The two regions are separated by a mobility edge E_c.[2,3] As analytic work is difficult, numerical calculations have been widely used in the study of Anderson localization. For a review see, e.g., Refs. 4 and 5.

In recent years, attention has been drawn to the quantum percolation problem. In classical percolation theory, a regular lattice is filled with particles with probability p and empty sites with probability $(1-p)$. Only connections between nearest neighbors are taken into account. There always exists a critical value p_c above which an infinite cluster appears in an infinite lattice. This is the classical percolation threshold. The present problem is called site percolation.[6]

In quantum percolation theory, the Anderson Hamiltonian is combined with classical percolation. A regular lattice is filled as described above and the ε and V parameters are defined as follows: ε_i is chosen to be zero for all i, $V_{ij}=1/Z$ if sites i and j are nearest neighbors and neither i nor j is an empty site; $V_{ij}=0$ otherwise. Z is the number of nearest neighbors. The Anderson transition point is called p_q. As long-range transport is only possible on the infinite cluster, p_q has to be larger than or equal to p_c, which is approximately 0.59 for the square and 0.31 for the simple cubic lattice.[6] Systems described by the same Hamiltonian have been studied by Kirkpatrick and Eggarter[7].

Most of the methods used in numerical studies of the Anderson problem are also used to obtain quantum percolation thresholds. Srivastava and Chaturvedi[8] have calculated the average inverse participation ratio by the equation-of-motion method of Weaire, Williams, and Srivastava.[9] Odagaki and Chang[10,11] have presented an approach based on a real-space renormalization-group analysis. Root, Bauer, and Skinner[12] have used a finite-size-scaling method to calculate p_q. The transfer-matrix method[13,14] has been used by Soukoulis, Economou, and Grest[15] to determine p_q and the mobility edge trajectory in three dimensions. Evangelou has studied the density of states and the inverse participation ratio in two and three dimensions.[16] Odagaki, Ogita, and Matsuda have obtained p_q for the square lattice by a Green's function method.[17] Raghavan and Mattis[18,19] have determined the quantum percolation thresholds by the recursion method.[20] This method has been frequently applied to the Anderson problem.[21] Meir, Aharony, and Harris have studied the quantum bond percolation problem by the inverse participation ratio.[22] Numerical estimates of quantum site-percolation thresholds range from 0.59 to above 0.94 for the square and from 0.38 to 0.70 for the simple cubic lattice.

II. METHOD

One measure of localization is the Thouless number. Thouless, Edwards, and Licciardello[23,24] (TEL) showed the proportionality between the conductivity of a system and the shift of the energy of an eigenstate as a result of changing boundary conditions from cyclic to anticyclic ones. The results are that

$$\sigma \propto N\langle \Delta E \rangle \rho(E) \tag{2}$$

in two dimensions, and

$$\sigma \propto N\langle \Delta E \rangle \rho(E)/L \tag{3}$$

in three dimensions. σ is the conductivity, $\langle \Delta E \rangle$ the geometric mean of the energy shift in an energy interval, $\rho(E)$ the density of states in that interval, N the total number of eigenstates, and L the length of the cube edge.

In the numerical work we proceed as follows: For each realization, the eigenvalues are calculated for cyclic boundary conditions and for Dirichlet boundary conditions. We have performed test calculations for both cyclic-anticyclic and cyclic-Dirichlet boundary conditions. The energy shifts showed no difference. As no crossing of eigenvalues as a result of changing boundary conditions should be allowed, the coupling strength between sites located at different edges of the system is kept small when cyclic boundary conditions are imposed. The coupling strength ranges from $\frac{1}{10}$ V to $\frac{1}{1000}$ V, depending on the particle concentration p. Whenever σ decreases with increasing system size, the states in the energy interval considered are dominantly localized states. The quantum percolation threshold is given by the concentration p below which this behavior is observed for all energy intervals. From the discussion above we also conclude that the averaging over an energy interval leads to a loss of information. We are looking for a transition where, for the first time, extended states appear. By averaging we can only conclude whether the states in an energy interval are dominantly localized. Even if the transition is sharp we smooth it out in this procedure. The method described above will be called the TEL method hereafter. As no eigenvectors are required for the TEL method, the systems studied with this method can be made very large.

To simplify the calculation, a basic symmetry property of the lattice can be exploited.[25] As the square lattice and the simple cubic lattice are bipartite, E_j and $-E_j$ are both eigenvalues of $\hat{H}$. As a result, only half of the eigenvalues have to be calculated. In addition, the symmetry of eigenvalues is an excellent test for the numerical accuracy in the algorithm used for the eigenvalue problem.

For the study of energy shifts as a result of different boundary conditions, a Hoshen-Kopelman algorithm[26] is used to grow the largest cluster on a lattice m^D. It is important to have only one cluster on the lattice to avoid the influence of many small clusters. Their presence may spoil the statistics, so all clusters but the largest have been eliminated. In the existing literature, this point has not always been properly accounted for. For the diagonalization we used the Lanczos algorithm.[27,28]

III. RESULTS

A. Results in three dimensions

For the simple cubic lattice, TEL calculations have been performed on an $8\times8\times8$, a $12\times12\times12$, and a $16\times16\times16$ grid with 50, 25, and 8 realizations, respectively.

With the help of Fig. 1 we explain how the quantum percolation threshold and the mobility edge are obtained. $\eta=-\log_{10}\sigma$ is plotted as a function of E for the occupation probabilities $p=0.35$, 0.45, and 0.55. The energy spectrum is subdivided into energy bins of width 0.0625. Within each energy bin, the behavior of η with increasing lattice size ($L=8$, 12, 16) is plotted from the left. Whenever η increases with increasing system size, i.e., σ decreases with increasing system size, the states in the energy interval considered are dominantly localized states. All bins showing this behavior are shaded. At $p=0.35$, all states are localized. At $p=0.45$ and 0.55, the spectrum can be subdivided into a part containing predominantly localized and a part containing dominantly extended states. For a given value of p we observe in general at high energies a decrease of η, i.e., an increase of σ, so this energy region contains dominantly extended states. For lower energies we observe an increase of η, i.e., a decrease of σ, so this energy interval contains dominantly localized states.

The regions of dominantly localized and dominantly extended states are separated by a mobility edge. This mobility edge has the value $E_c\approx0.4$ for $p=0.45$ and

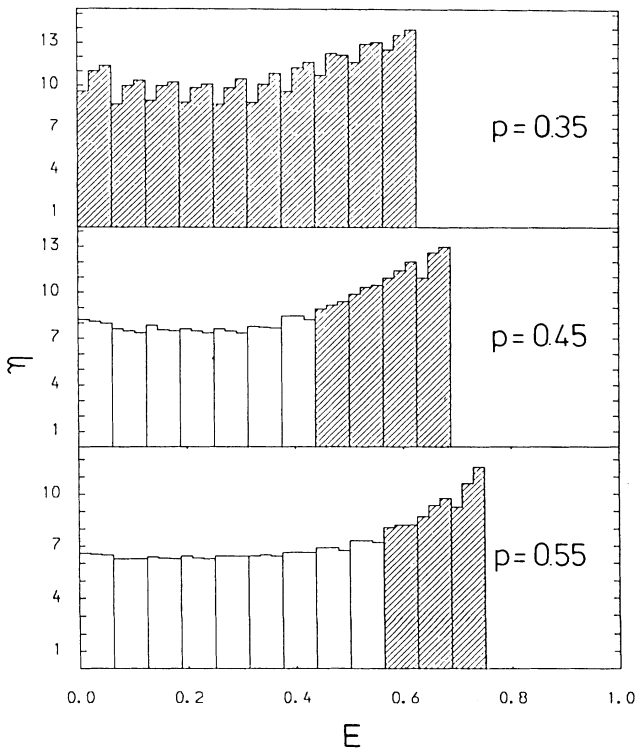

FIG. 1. $\eta=-\log_{10}\sigma$ as a function of E for the simple cubic lattice for $p=0.35$, 0.45, and 0.55. For details, see text. η and E in arbitrary units.

$E_c \approx 0.56$ for $p = 0.55$. The mobility edge trajectory, i.e., E_c as a function of p, can be obtained by calculating E_c for a number of different p values. This has been done for the p values indicated in Fig. 2. The mobility edge calculated by Soukoulis, Economou, and Grest[15] is contained in Fig. 2 as well. At $p = 0.45$, intervals containing extended states can be observed for the first time. It is thus concluded that p_q equals 0.45. As the fluctuations of the ΔE values are large, p_q can only be determined within a certain range of the occupation probability. We estimate this to be 0.45 ± 0.03 from detailed calculations of occupation probabilities in the neighborhood of 0.45.

We observe that the opening of the region which contains dominantly extended states is rather sudden. Below $p = 0.45$ all states appear to be localized for all energies, and at $p = 0.45$ a wide energy interval (from $E \approx -0.44$ to $E \approx +0.44$) opens suddenly in which we find dominantly extended states. Due to the statistics of the present calculations it is impossible to derive an analytic form for the mobility edge as a function of the occupation number.

The total width of the density of states increases with increasing value of the occupation probability p. At $E = 0$ the density of states has a spike. This spike increases with decreasing p. It is separated from the remainder of the density of states by a small gap. The density of states is shown for three different values of p in Fig. 3. The spike at $E = 0$ is suppressed. According to Kirkpatrick and Eggarter,[7] this spike is caused by localized states with a high local symmetry. They may occur even on a large, finite cluster. Figure 3 also shows the mobility edge obtained with the TEL method. The part of the spectrum which is dominated by localization is shaded.

B. Results in two dimensions

For the square lattice, the TEL method is applied to systems containing at least 512 and 1024 particles with 50 and 25 realizations, respectively. The quantum percolation threshold and the mobility edge trajectory are obtained as described in Sec. II. p_q equals 0.70, and a plot of the mobility edge trajectory is presented in Fig. 4.

To avoid a numerical problem described below, a different coupling strength γ is chosen for systems with a different occupation probability p. A large value of p causes a large energy shift ΔE, so the coupling strength is

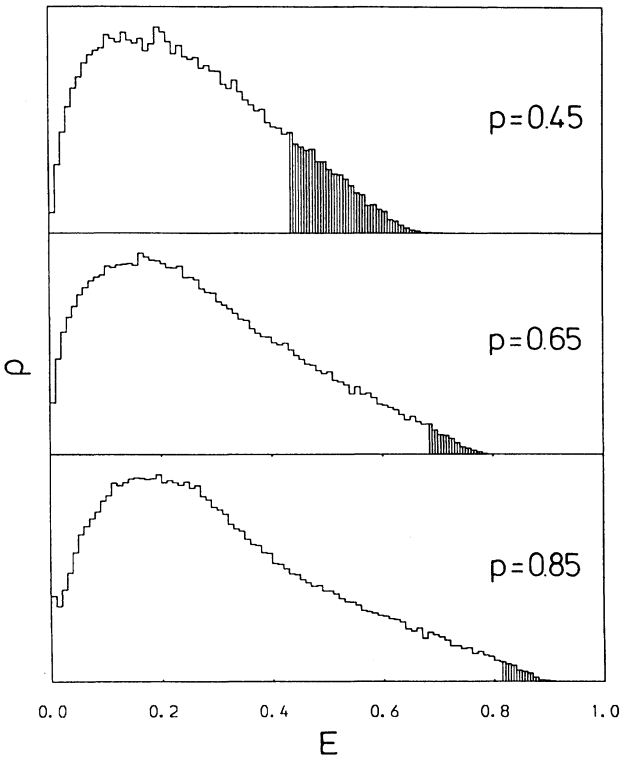

FIG. 3. Density of states for the simple cubic lattice for $p = 0.45$, 0.65, and 0.85; ρ and E in arbitrary units. The localized part of the spectrum is shaded.

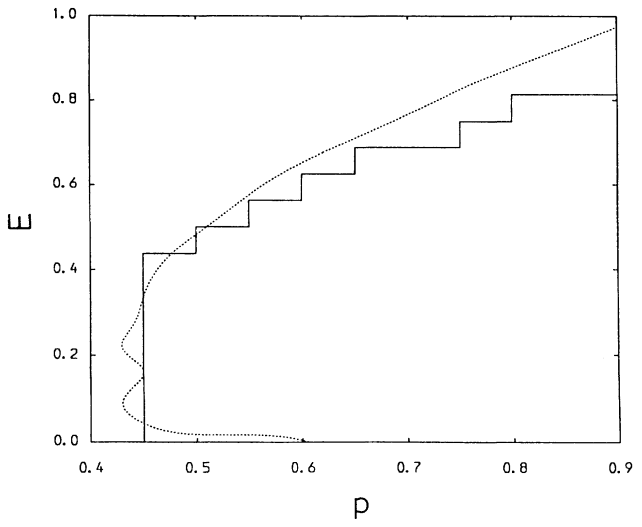

FIG. 2. Mobility edge trajectory for the simple cubic lattice. Dotted line: mobility edge trajectory obtained by Soukoulis, Economou, and Grest (Ref. 15). E in arbitrary units.

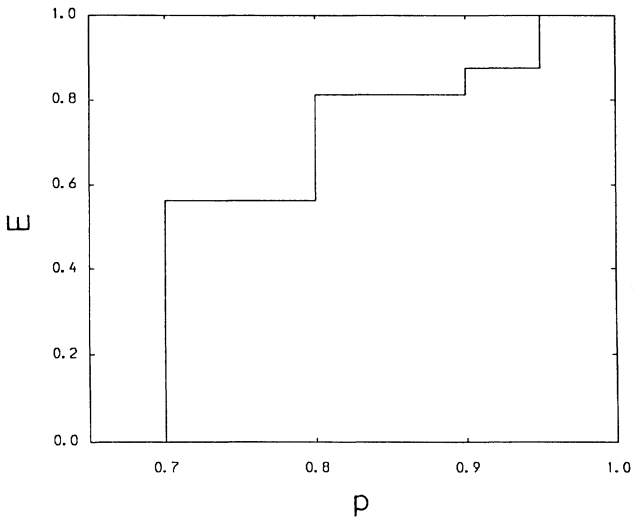

FIG. 4. Mobility edge trajectory for the square lattice. E in arbitrary units.

kept small. If $p < p_q$, the energy shift $\langle \Delta E \rangle$ may be smaller than the accuracy obtained with the eigenvalue algorithm, so the results may become meaningless. In this case γ is increased up to $\frac{1}{10}V$ to enlarge $\langle \Delta E \rangle$. No problems of this kind are observed for the simple cubic lattice, where we have chosen $\gamma = \frac{1}{1000}V$. The density of states shows the same features as the density of states in three dimensions.

IV. DISCUSSION

Literature results for quantum percolation thresholds are collected in Table I. The situation is as follows. In three dimensions p_q ranges from 0.38 to 0.70. All calculations based on a scaling hypothesis or related approaches, i.e., the work of Chang and Odagaki,[10,11] Root, Bauer, and Skinner[12] and Soukoulis, Economou, and Grest,[15] lead to $0.42 \leq p_q \leq 0.48$ with one exception. An early work of Chang and Odagaki,[10] based on a real-space renormalization approach, gives a value of 0.70 for p_q. The method has been applied to larger systems by the same authors,[11] correcting this value which then became 0.42.

The TEL method used in this work is closely related to scaling methods, because a quantity proportional to the conductivity σ is studied as a function of the system size. Thus our result, $p_q = 0.45$, falls into the expected range. According to Licciardello and Thouless,[24] the inverse localization length κ of an exponentially localized eigenfunction can be obtained by

$$\kappa = \frac{1}{\lambda} = -\frac{d \ln \sigma}{dL} \quad . \tag{4}$$

As we have studied systems of only three different sizes in three dimensions and two different sizes in two dimensions, we can neither decide whether an eigenfunction obeys an exponential or a power-law decay nor calculate the localization length quantitatively. Nevertheless, it can be seen (Fig. 1) that for a given p the localization length is small at the band edge and large near the mobility edge.

Raghavan[19] has calculated the quantum percolation threshold by an application of the recursion method,[20] giving $p_q = 0.38$, which is close to the smallest value obtained with a renormalization approach ($p_q = 0.42$).[11]

The mobility edges calculated with the TEL method and with the transfer-matrix approach of Soukoulis, Economou, and Grest[15] almost coincide. The Anderson transition occurs in a large energy interval at $p = 0.45$ and the mobility edge is moving towards the band edge as p increases. There always exists a mobility edge up to $p = 0.90$. Soukoulis, Economou, and Grest[15] have observed a narrow mobility gap at $E = 0$. We think that this gap is caused by the unique localization properties of eigenfunctions at $E = 0$. According to Kirkpatrick and Eggarter,[7] all of these states are localized due to a high local symmetry. As our TEL calculation gives nearly the same p_q value and the same mobility edge trajectory as the work of Soukoulis, Economou, and Grest,[15] it supports their choice of the localization length divided by the system size, $\lambda_M / M = 0.6$, to identify the mobility edge.

In two dimensions, the literature results for p_q range from 0.59 to above 0.94 and so almost cover the entire possible interval $[p_c = 0.59, 1.0]$. Using the TEL method, we obtain $p_q = 0.70$. The mobility edge trajectory looks similar to the one calculated for the cubic lattice: There is a large energy interval in which the Anderson transition occurs, and then the mobility edge moves gradually towards the band edge.

The methods used in the literature to calculate p_q for the square lattice are described above. Dropping the p_q value of the first work of Odagaki and Chang (see above) and $p_q = p_c$, the results can be grouped as follows: (i) p_q is close to one.[11] This value is supported by similar results for the quantum bond percolation problem.[22] (ii) p_q is close to 0.7, as obtained by Srivastava and Chaturvedi[8] and our TEL calculation. Raghavan[19] has calculated a rather broad interval for p_q, ranging from 0.7 to 1.0.

A similar contradiction has been discussed for the Anderson problem.[4] The numerical results give either $W_c / V \approx 6$ or $W_c / V = 0$ for the square lattice, depending on the system size and on the method used. Numerical applications of the scaling theory of localizations[13] lead to $W = 0$, and the equation-of-motion method[9] leads to $W \approx 6$. Results obtained with the TEL method depend on the system size.[23,24] For small systems, $W_c \approx 6$, whereas for large systems there are serious doubts about the existence of an Anderson transition above $W = 0$. It

TABLE I. Results for the quantum site-percolation problem. The abbreviations used are as follows: RG, renormalization group; GF, Green's function method; RM, recursion method; EOM, equation of motion; TEL, method of Thouless, Edwards, and Licciardello; TM, transfer-matrix method; 2D, two dimensional; 3D, three dimensional.

Author(s)	Reference	Method	p_q (2D)	p_q (3D)
Chang and Odagaki	11	RG	≥ 0.94	0.42
Odagaki and Chang	10	RG	0.87	0.70
Oagaki, Ogita and Matsuda	17	GF	0.59	
Raghavan	19	RM	0.70–1.0	0.38
Root, Bauer, and Skinner	12	RG		0.48
Soukoulis, Economou, and Grest	15	TM		0.44
Srivastava and Chaturvedi	8	EOM	0.73	0.47
This work		TEL	0.70	0.45
p_c	6		0.59	0.31

is interesting to note that those methods applied to both the Anderson problem and the quantum percolation problem lead to the same transition behavior (either a transition at arbitrary weak disorder or a transition at finite disorder) for both problems. All of these methods give a unique result for p_q in three dimensions.

According to the analytical scaling theory of localization,[29] no extended states should occur for any amount of disorder in two-dimensional systems. A transition from a weakly localized to a strongly localized behavior is allowed, however. So the result $W_c/V \approx 6$, can be interpreted as the point of transition from a weakly to a strongly localized behavior. Strongly localized states show an exponential spatial decay, whereas the decay of weakly localized states obeys a power law.

We suggest similar localization properties for the quantum percolation problem on the square lattice: A transition from weakly to strongly localized states occurs at $p_q' = 0.7$ and a transition from extended to weakly localized states at $p_q = 1.0$. The type of transition obtained is determined by the method or the system size used in the calculation. As we use rather small lattices in the TEL approach, we obtain the first kind of transition. Further calculations with different methods, e.g., the transfer-matrix approach, should be performed for two-dimensional lattices to resolve the problem.

V. CONCLUSIONS

We have studied the quantum percolation problem numerically for large systems on the square lattice and on the simple cubic lattice. Quantum percolation thresholds and mobility edge trajectories have been calculated by the behavior of a number proportional to the conductivity as a function of the system size, leading to $p_q = 0.45 \pm 0.03$ in three dimensions and $p_q = 0.70 \pm 0.03$ in two dimensions.

For the simple cubic lattice, the mobility edge trajectory has been calculated for the first time without making any assumptions about a critical localization length. The mobility edge appears to open up rather suddenly at $p_q = 0.45$ over a broad energy interval and then moves slowly towards the band edge. Except for the states at $E = 0$, which play a special role, there does not appear to be a mobility gap at $E = 0$.

To resolve an uncertainty about the value of p_q for the square lattice in the existing literature, we have suggested the existence of two transitions in two dimensions, according to a similar behavior observed for the Anderson problem in two dimensions. A transition from weakly to strongly localized states occurs at $p_q' = 0.7$ and a transition from extended to localized states occurs at $p_q = 1.0$

For the square lattice, the mobility edge trajectory separating weakly and strongly localized states has been calculated. The mobility edge trajectory opens up suddenly at $p_q = 0.70$ similar to the mobility edge trajectory calculated for the simple cubic lattice.

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