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# Quantum percolation and the Anderson transition in dilute systems

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Computer-simulation results are presented for quantum systems with discrete off-diagonal disorder in square and cubic lattices. For the quantum percolation model with bonds present or absent at random the density of states shows a dip at the band center which develops into a gap for strong dilution. The relation between the quantum and geometrical percolation thresholds $p_q > p_c$ is satisfied for these lattices as well as for Cayley trees. In a model with alternating sign of bonds, most of the states in the band remain delocalized.

Considerable progress has been made[1] in our understanding of the Anderson transition between localized and extended states in a disordered quantum system. Complete localization is predicted for $d \leq 2$ with the occurrence of a transition above two dimensions with mobility edges $E_c$ emerging in the band separating localized from extended states. The "critical" behavior near $E_c$ is established in terms of field-theoretic expansions in $\epsilon = 2 + d$.[2] However, the commonly studied case is that of diagonal disorder in which the site energies of a single-particle Hamiltonian on a periodic lattice are stochastic variables. Less attention has been paid to *off-diagonal disorder* where, instead, the hopping elements vary at random.[3] Randomly dilute lattice systems have also attracted a lot of attention recently.[4] In this case the disorder can manifest itself in both the geometrical and quantum aspects of the model and one expects a classical percolation as well as an Anderson transition. In this Communication a simple numerical simulation study is presented of the *quantum bond percolation model* brought into attention by Raghavan and Mattis,[4] although a related site model was studied much earlier by Kirkpatrick and Eggarter.[5] A different model with a discrete type of disorder is also considered as a special case of the *random-phase model* proposed by Sadovskii.[6] This work was in part motivated by the existence of amorphous materials with short-ranged off-diagonal interactions of a common sign, such as amorphous semiconductors[7] and spin-glasses with alternating sign.[8]

The quantum-mechanical single-particle Hamiltonian in a tight-binding form is

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} |i\rangle \langle j| \ , \tag{1}$$

using an orthogonalized site representation in a $d$-dimensional lattice. The hopping integrals, which differ from zero only between nearest neighbors, are assumed to be random quantities chosen from a probability distribution. For the quantum percolation model the randomness refers to the modulus of $J_{ij}$ so that

$$P(J_{ij}) = p\delta(J_{ij} - 1) + (1 - p)\delta(J_{ij}) \ , \tag{2}$$

and bonds are present or absent in a lattice with probability $p$ and $1 - p$, respectively. For the other model considered, $J_{ij} = \exp(i\Phi_{ij})$ and the phase $\Phi_{ij}$ is instead the independent random variable. In the dilute case "antiferromagnetic" bonds are introduced at random by

$$P(J_{ij}) = p\delta(J_{ij} - 1) + (1 - p)\delta(J_{ij} + 1) \ . \tag{3}$$

It can be shown that the Hamiltonian (1) with (3) is invariant under a local gauge transformation defined in Ref. 6, and the concept of frustration can be introduced for the electronic system in analogy with spin-glasses.[8] It is known from percolation theory that for $p > p_c$, the percolation threshold, an infinite cluster appears which covers the whole lattice as $p \to 1$. The Anderson transition, at which *all* states of (1) on the percolating become localized, occurs at a probability $p_q$, and the inequality $p_q > p_c$ was recently found to hold. Raghavan and Mattis[4] approached the problem from the "pure limit" ($p = 1$) by using the well-suited method of tridiagonalization, while Shapir *et al.*[9] developed series expansions in powers of $p$ for a range of dimensions. These authors find indications of complete localization, $p_q \simeq 1$ in $d = 2$ in accordance with the scaling theory,[1] and $p_q \simeq 0.37$ (Ref. 4) or 0.32 (Ref. 9) in $d = 3$, which may be compared with $p_c = 0.50$ and 0.256 in $d = 2$ and 3, respectively. In this Communication localization is studied by a more direct numerical procedure. The complete eigensolutions are obtained numerically for many random samples of square lattices up to $64 \times 64$ and cubic lattices of $10 \times 10 \times 10$ with periodic boundary conditions in all directions.[10] The present work can be regarded as complementary to that of Refs. 4 and 9 as well as a check of their results, via independent means, when their range of validity coincide.

The configurationally averaged *density of states*

 

$\rho(E)$ is an even function of the energy $E$ as a consequence of the dual interconnected sublattice structure of the lattices considered. For $p=1$, $\rho(E)$ is nonvanishing in the range $[-Z,Z]$, where $Z=2d$, and for $p<1$ the band narrows for the distribution (2) and has total weight $p$ states per site. Dilution of this sort is expected to create strong local disorder in special parts of the percolating cluster leading to highly localized states known as Kirkpatrick-Eggarter localization, which contribute to spikes in $\rho(E)$.[5] These $\delta$-function singularities occur precisely at certain special energies, e.g., 0, $\pm 1$ in $d=2$ and 0, $\pm 1$, $\pm\sqrt{2}$ in $d=3$, and they are partly due to isolated clusters. Moreover, these states are highly degenerate and can coexist with extended states.[5,9]

We have calculated densities of states for large systems and many random samples. The dip is observed at the band center for concentrations higher than $p_c$ unaffected by size variation or the number of samples (see Figs. 1 and 2 ), although the infinitesimal gap in the inset is most probably a finite-size effect. We find no indication of dips at other special energies in our samples for moderate concentrations. Effective-medium theories, reproduce the dip and the gap with a $\delta$ function at the origin, but at much lower $p(\leq 1/Z)$.[11] For the distribution (3) the effect of dilution is much less drastic and $\rho(E)$ differs little from the pure case except at the band edges where it becomes smoothed.

The chief concern of this Communication is *the question of localization* although we do expect this to be associated with the anomalies in $\rho(E)$. The definition of mobility edges has to be modified in this case so that they separate extended and possible coexisting localized states from purely localized states. We have calculated the inverse participation ratio (IPR) defined by

$$y(E)=\sum_i \psi_E^4(i) \ ,$$

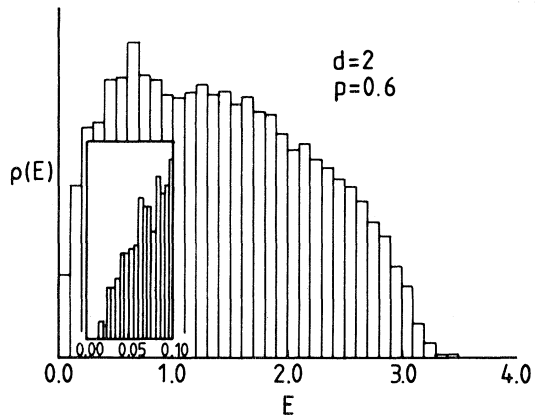


FIG. 1. Density of states, $\rho(E)$ $[=\rho(-E)]$, for quantum percolation averaged over 20 configurations in $32\times 32$ and $64\times 64$ square lattices. The dip at the band center is displayed and a $\delta$-function singularity exists at $E=0$.

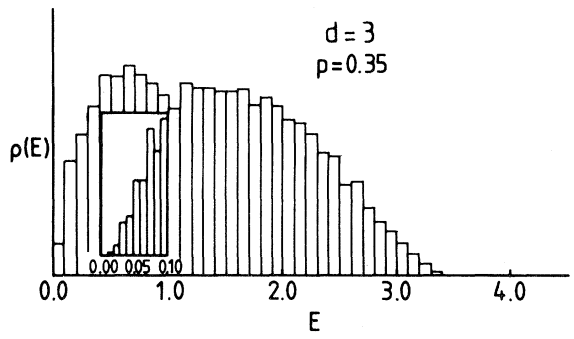


FIG. 2. Same as in Fig. 1 but for $10\times 10\times 10$ cubic lattices.

for each normalized eigenvector $\psi_E$. The use of $y(E)$ is expected to probe directly the spatial extent of the eigenstates and can also indicate the position of $E_c$. For an extended state, $y(E)$ is expected to be very small, of about $3/N$ for $N$ sites, while localized states show higher $y(E)$ values. In $d=3$ we observe no extended states up to $p_q\simeq 0.35$, which confirms the estimates of Refs. 4 and 9 (Fig. 3). In $d=2$ (Fig. 4) the situation is more complicated but, for $p=0.6$, $y(E)$ shows localized behavior for all the eigenfunctions on the percolating cluster. Our main concern is to examine states other than at special energies where localized states also occur; therefore we do not expect this degeneracy to affect our results.[9] The safe conclusion $p_q>p_c$ can be reached on the basis of this calculation in $d=2$ and 3. We also find an indication that in $d=2$ the behavior of the localization length closely resembles the corresponding behavior in the original Anderson model.[1] For the random-phase model (3) extended states appear at every concentration in agreement with Sadovskii.[6] It must be emphasized that phase disorder introduced via (3) is nontrivial and cannot be eliminated by a suitable gauge transformation apart from $d=1$. In $d=2$ and 3 complete randomization of the phases may occur[6]; however, even in this case, only about $\frac{1}{3}$ of the states in the band are probably localized (Fig. 5).[12]

Finally, the case of the *Cayley tree* of connectivity $K(=Z-1)$ is considered, which is regarded as a pseudolattice with no closed loops but maps exactly into a real $d$-dimensional lattice in the cases of $K=1$ $(d=1)$ and $K=\infty$ $(d=\infty)$. The conclusions drawn previously are supported by recent exact calculations on Cayley trees by Harris[13] and Thouless and Kirkpatrick,[14] since in this limit the Anderson transition is well understood.[15] A different approach is used in this case in order to check these analytical calculations of $p_q$ which give different results, e.g., for $K=2$, $p_q=0.59$ (Ref. 13) and 0.75 (Ref. 14), compared with $p_c=0.5$ $(=1/K)$. I have calculated the tridiagonalization coefficients $b_n$ for many random samples going up to 10–15 steps in connected trees with no closed loops, corresponding to $K=2$. A lo-

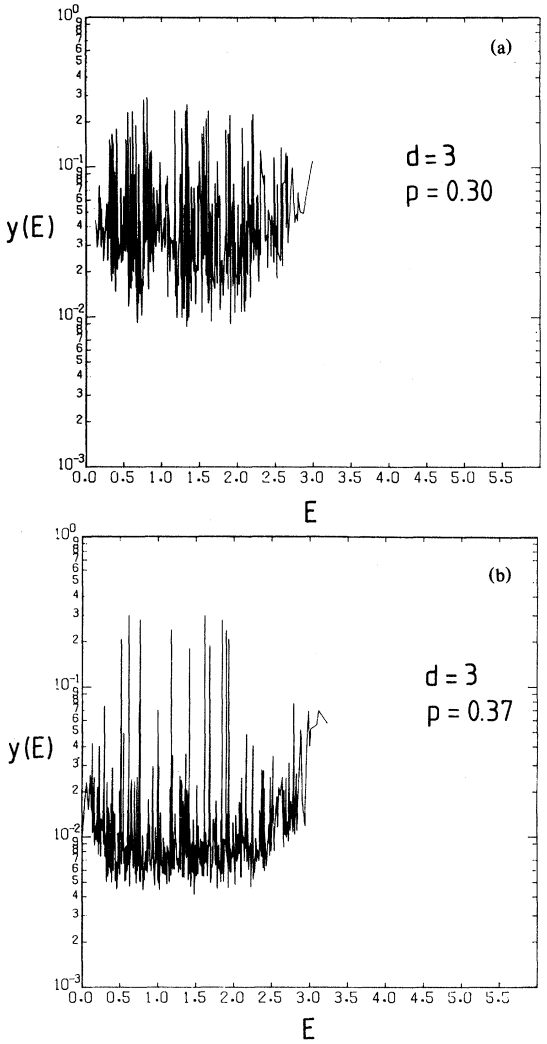


FIG. 3. IPR for the quantum percolation model in cubic $10 \times 10 \times 10$ lattices. The highly localized states [large $y(E)$] are partly due to isolated clusters and partly to special parts of the percolating cluster. In case (a) all states are localized while extended states [ $Y(E)$ of the order $O(10^{-3})$] coexist with localized states.

calization criterion defined in Ref. 4 is related to the measure of the noise in $b_n$'s. The asymptotic value of this noise $\Delta$ is 0.28 for $p=0.5$, 0.23 for $p=0.6$, 0.13 for $p=0.7$, and 0.09 for $p=0.75$, while for $p>0.75$ the $b_n$'s converge within an uncertainty of less than $\pm 0.05$. This leads to qualitative agreement with both estimates of $p_q$. Difficulties are encountered in this simulation approach similar in nature to those experienced in Ref. 15; however, within the quoted uncertainty, the tridiagonalization favors a $p_q=0.75$ in agreement with Ref. 14. For the model (3), within the same method, it can be trivially shown that all the states remain extended, perhaps due to the lack of frustration.

In conclusion, I have presented numerical results

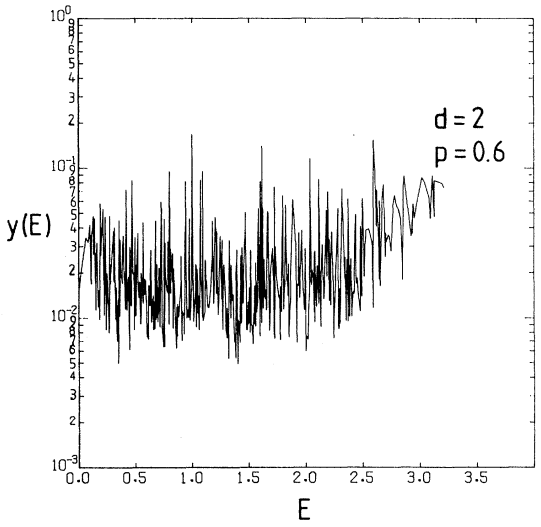


FIG. 4. IPR for the $32 \times 32$ square lattice but with the isolated clusters removed in this case.

which confirm earlier estimates of $p_q$ in $d=2$, 3 as well as the Cayley tree and demonstrate the essential features of the density of states $\rho(E)$, similar to those found in Ref. 5. The behavior of $\rho(E)$ at the band center with a dip or a gap present in $d=2$, 3 must be exclusive to quantum percolation models since, for *continuous randomness* of positive sign in $d=2$, the singularity at $E=0$ probably takes the Dyson form $\rho(E) \sim 1/E|\ln E|^3$ (Ref. 16) for strong disorder while, for continuous gauge invariant models,[17] $\rho(E) \sim \ln(1/|E|)$, and no singularity exists in $d=3$. There are still many questions left to be answered, particularly concerning a more sensitive calculation of $p_q$ in the marginal $d=2$ as well as the localization of spin-wave excitations.

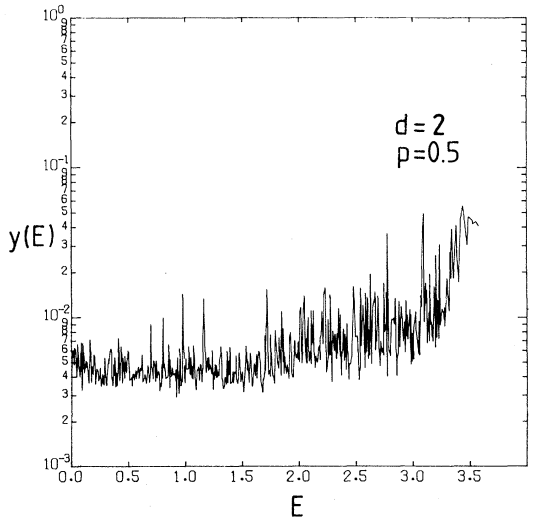


FIG. 5. IPR for the random-phase model (3). A mobility edge could be located between $E=2.0$ and 2.5.

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