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New scaling results in quantum percolation

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Computer simulations are reported for the average number of lattice sites falling under a localized wave function as a function of concentration for a model binary system with "infinite disorder." Novel structures are found near classical and quantum percolation thresholds which are explained using scaling arguments. It is also pointed out that extended states may appear even at infinite disorder in two-dimensional binary systems.

Classical percolation provides a useful framework for obtaining an intuitive understanding of Anderson localization in *binary systems*.[1] This analogy, however, does not hold in a strict sense. Localization being a quantum-mechanical phenomenon, conduction sets in when an extended state is formed.[2-5] This we take as the definition of "quantum percolation." A striking feature of this model is that as extended state appearing at the quantum-percolation threshold, x_q cannot be destroyed even by infinite disorder.[2,3]

A direct estimation of localization is done in terms of "inverse participation number," $\mathscr{P}$, the inverse of number of lattice sites participating in a wave function. We report numerical simulation results for $\mathscr{P}$ in two- and three-dimensional systems using equation of motion method.[3,6,7] Novel features are found near classical and quantum percolation thresholds. Plausible interpretation is given using scaling arguments.

COMPUTER SIMULATION FOR $\mathscr{P}$ IN QUANTUM PERCOLATION FRAMEWORK

We work with the Hamiltonian

$$H_{AA} = \sum V |i\rangle \langle j| \ , \tag{1}$$

which mimics a system with infinite disorder; V, the hopping integral between atoms of type A situated at nearest-neighbor sites i and j, takes a fixed value. The states are confined to A sites only and the other type of atoms are formally removed from the picture. In such a system we shall

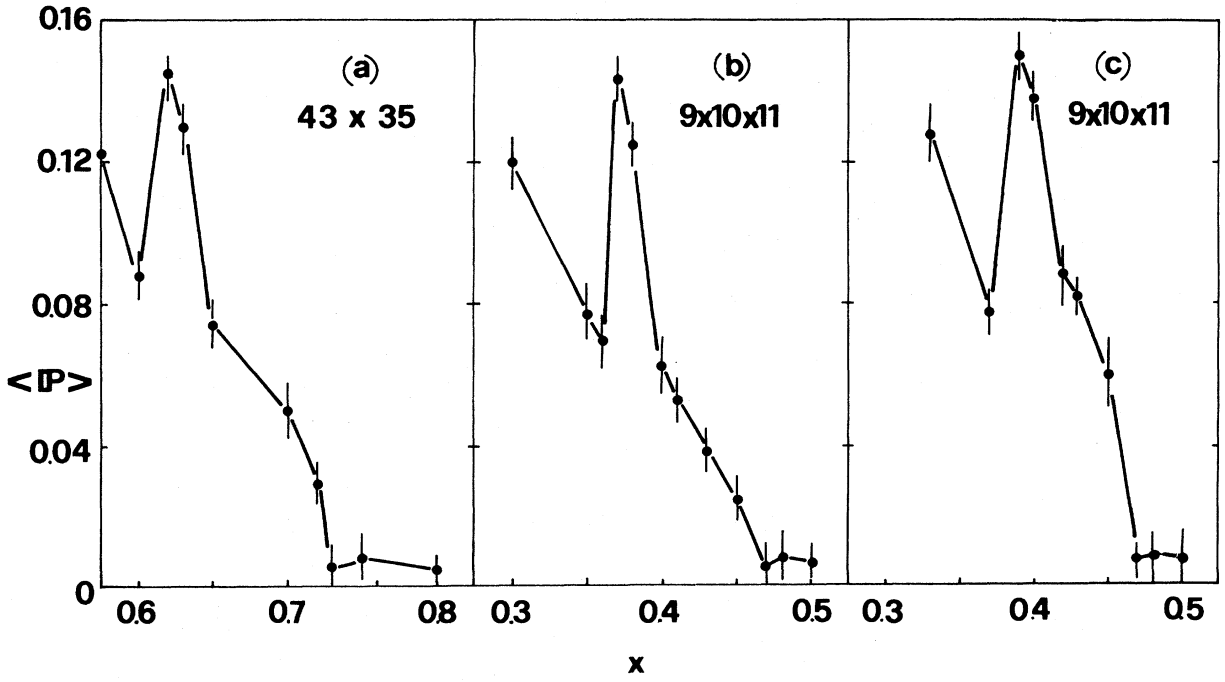

FIG. 1. Computer simulation results for (a) square and (b) and (c) cubic lattices. (b) and (c) are obtained using different random number generators. Points in the uninteresting region, $x < x_c$, are not shown—monotonic decrease is found.

study the effect of increasing concentration x of A atoms. We shall denote by x_c, the percolation threshold at which an open cluster of A atoms connected by nearest-neighbor bonds is formed in an infinite system, and by x_q, the quantum-percolation threshold defined above.

The numerical method used is described in Refs. 3 and 6. It involves the calculation of the time dependence of a random trial-wave function and yields averages of the quantity

$$\sum_i^N |\psi_i|^4 \Big/ \left[\sum_i^N |\psi_i|^2\right]^2 , \tag{2}$$

where ψ is an eigenfunction and the summations are over all sites. This is N^{-1} times the inverse participation *ratio*, i.e., $\mathscr{P}$. Band averages of (2), denoted by $\langle \mathscr{P} \rangle$ are related to time averages of a suitably chosen random wave function, according to[7]

$$\langle \mathscr{P} \rangle = (N/2) \sum_i^N (2\bar{Q}_i^2 - \bar{Q}_i^2) , \tag{3}$$

where $\bar{Q}_i$ is the time-averaged probability associated with site i. In $\langle \mathscr{P} \rangle$ we have used polynomial weighting about the center of the band.[6] Results for fairly large square and cubic lattices are shown in Fig. 1. Two dips are seen which should be attributed to x_c and x_q. A sharp rise just above x_c is found which attains a maximum followed by a sharp fall to a minimum. After this minimum there is a small tendency to rise or to remain almost constant. We find $x_c = 0.59$ and $x_q = 0.73$ for square lattice, and for cubic lattice $x_c = 0.37$ and $x_q = 0.47$. The values for x_c are in very good agreement with earlier results,[8] in particular the value for square lattice.

INTERPRETATION OF FEATURES IN $\mathscr{P}$

We shall study three successive regions ($x < x_c$; $x_c \leqslant x < x_q$; $x \geqslant x_q$) individually.

(i) $x < x_c$. The wave function is confined entirely to finite, isolated clusters of sites. States of energies near the center of the band will have comparable amplitudes throughout the finite cluster; they would be extended but for the limitation to the extent of the cluster. This should be understood as follows. The only tendency towards localization of a state to part of the cluster comes from those sites with reduced coordination number. This forces the energies of states of large amplitude on such sites towards the center of the band where they will overlap in energy with states associated primarily with sites of higher coordination, reducing the tendency towards localization beyond that required by the cluster size. Thus $\langle \mathscr{P} \rangle$ for a given cluster is the inverse of the cluster size ν, where $\langle\ \rangle$ denotes average over band energies. $\langle \mathscr{P} \rangle$ for the entire sample is given by

$$\langle \mathscr{P} \rangle = \int \nu^{-1} w(\nu) d\nu , \tag{4}$$

where $w(\nu)$ is the cluster size distribution normalized to one. As x_c is approached, more and more of $w(\nu)$ is pushed towards large ν until at x_c the mean cluster size diverges,

$$\int \nu w(\nu) d\nu \propto (x_c - x)^{-\tau}; \quad x \to x_c^- . \tag{5}$$

Consequently, the integral in (2) decreases monotonically as $x \to x_c^-$ but remains finite at x_c.

(ii) $x_c \leqslant x < x_q$. Above x_c there is an infinite cluster. The fraction of sites in the infinite cluster, P_p^c, is the percolation probability. The normalization of $w(\nu)$, which refers to finite clusters only, is now

$$\int w(\nu) d\nu = 1 - P_p^c . \tag{6}$$

The percolation probability grows monotonically with increasing $x (> x_c)$,

$$P_p^c \propto (x - x_c)^{\beta}; \quad x \to x_c^+ . \tag{7}$$

It is convenient to introduce a normalized cluster size distribution for $x > x_c$,

$$v(\nu) = w(\nu)/(1 - P_p^c); \quad \int v(\nu) d\nu = 1 . \tag{8}$$

Classically, the infinite cluster does not contribute to $\langle \mathscr{P} \rangle$. However, quantum mechanically the states in infinite cluster may be localized for various reasons.[1,4] Denoting by ν_L the number of sites under the localized wave functions in the *infinite cluster* and assuming a normalized distribution $W(\nu_L)$, we can write $\langle \mathscr{P} \rangle$ as

$$\langle \mathscr{P} \rangle = (1 - P_p^c) \int v(\nu) \nu^{-1} d\nu + P_p^c \int W(\nu_L) \nu_L^{-1} d\nu_L . \tag{9}$$

As x increases above x_c, the larger clusters merge with the infinite cluster. The weight in $v(\nu)$ shifts down towards smaller clusters, whereas the weight in $W(\nu_L)$ shifts towards larger localized states until an extended state appears at x_q, i.e.,

$$\int v(\nu) \nu \, d\nu \propto (x - x_c)^{-\tau'}; \quad x \to x_c^+ , \tag{10}$$

and

$$\int W(\nu_L) \nu_L \, d\nu_L \propto (x_q - x)^{-\omega}; \quad x \to x_q^- . \tag{11}$$

Thus the second factor in the first term on the right-hand side of (9) increases singularly in a monotonic fashion with x as the mean size of the finite cluster decreases; the first factor $(1 - P_p^c)$ remains close to unity for x near x_c but monotonically decreases with increasing x. The second term decreases monotonically to a finite value at x_q^-. Thus there is a maximum at some $x > x_c$.

(iii) $x \geqslant x_q$. At x_q an extended state appears in the infinite cluster. A fraction P_p^q of the sites in the infinite cluster falls under the extended state and is defined as quantum-percolation probability. The normalization of $W(\nu_L)$, which pertains to localized states (in the finite cluster) only, is now

$$\int W(\nu_L) d\nu_L = 1 - P_p^q .$$

The P_p^q grows monotonically with increasing $x > x_q$ like

$$P_p^q \propto (x - x_q)^{\beta_q}; \quad x \to x_q^+ . \tag{12}$$

The normalized size distribution for localized states in infinite cluster for $x > x_q$ is

$$V(\nu_L) = W(\nu_L)/(1 - P_p^q); \quad \int V(\nu_L) d\nu_L = 1 .$$

Thus $\langle \mathscr{P} \rangle$ is finally given by

$$\langle \mathscr{P} \rangle = (1 - P_q^c) \int v(\nu) \nu^{-1} d\nu + (1 - P_p^q) P_p^c \int V(\nu_L) \nu_L^{-1} d\nu_L . \tag{13}$$

The first term, after having shown a peak at some $x > x_c$, is now dercreasing monotonically for $x > x_q$. In the second term the weight in $V(\nu_L)$ shifts down towards smaller localized states, i.e.,

$$\int V(\nu_L)\nu_L \, d\nu_L \propto (x - x_q)^{-\omega'}; \; x \to x_q^+ \; . \tag{14}$$

Following similar arguments which were applied to the first term in (9), we would expect another maximum at some $x > x_q$. This maximum is expected to be weak because (a) the overall magnitude of $\langle \mathscr{P} \rangle$ shall be small at such large values of x and (b) the probability of finding *small* localized states in greatly swollen infinite cluster shall be very small.[4] Putting all of this together, we have obtained the following results for $\langle \mathscr{P} \rangle$ which are also depicted schematically in Fig. 2:

(1) $x < x_c$: a monotonic decrease due to growing cluster size; (2) $x = x_c$: a minimum due to "divergent" mean cluster size; (3) $x \gtrsim x_c$: an initial increase due to decreasing mean cluster size of finite clusters; (4) $x > x_c$: a maximum and subsequent decrease due to infinite cluster containing an increasing number of sites. Localized states in the infinite cluster contibute to $\langle \mathscr{P} \rangle$ and add to its magnitude which is otherwise steadily falling; (5) $x = x_q$: another minimum due to divergent mean size of localized states; (6) $x > x_q$: a slow decrease for a weak maximum at $x \simeq x_q$. This is in excellent agreement with what the simulations have revealed in the previous section.

The peaked structure in $\langle \mathscr{P} \rangle$ should show up in an experimental study on conductivity as a function of concentration. They may prove to be of significance in metal-oxide-semiconductor (MOS) devices.[9] It may be interesting to calculate the exponent β_q and connect it to the conductivity exponent.[5,10] The observed structure may yield further insight into the percolative approach to spin glasses and the recent novel studies on superconducting networks.[11]

Attention should be paid to the low value of x_q for square lattice which may be significant in connection with the controversy[12] over complete localization in two-dimensional systems at small disorder. Tendency towards localization keeps $\langle \mathscr{P} \rangle$ large and formation of extended states or very large localized states reduces the magnitude of $\langle \mathscr{P} \rangle$. If we exclude the possibility of extended states and very large localized states, then P_p^q will be nearly zero and we will expect a monotonic decrease in $\langle \mathscr{P} \rangle$ after the maximum at $x \simeq x_c$ to a negligible value at $x \simeq 1$ (shown by dash-dot line in Fig. 2). But the numerical calculations show a large departure from this behavior; $\langle \mathscr{P} \rangle$ instead steeps down to a very small value much earlier than $x = 1$. This could indicate either that extended states have appeared, or that very large localized states are formed at x_q which grow in size as the size of infinite cluster grows for $x > x_q$ but are never converted into real extended state. The difference between the two possibilities would be beyond the scope of numerical simulation to detect. However, while one could imagine the latter to be possible at very large disorders, it would be strange if it happens at *infinitesimal* disorders over a large concentration range (70–100%). Thus our results showing extremely small values of $\langle \mathscr{P} \rangle$ for $x > x_q$ do not favor complete localization at very small disorders.

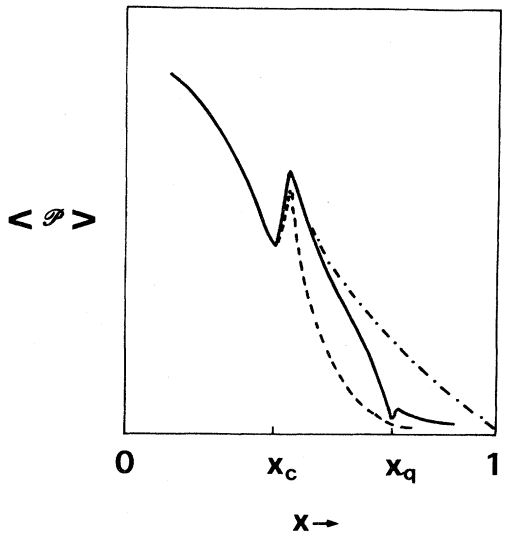

FIG. 2. Schematic plot of $\langle \mathscr{P} \rangle$ vs x as expected from Eq. (13): Dashed line denotes classical contribution coming from the first term in Eq. (13). The difference between dashed line and solid line is the contribution coming from localized states in the infinite cluster. Dash-dot line is for the case when $P_p^q = 0$.

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