RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 30, NUMBER 3 1 AUGUST 1984

Real-space renormalization-group analysis of quantum percolation

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(Received 26 March 1984)

Quantum percolation problems are studied with the use of a real-space renormalization-group method. A quantum effect is taken into account by calculating the quantum-mechanical efficiency of the Kadanoff cell in opening a channel for an electron in the cell. The quantum percolation threshold and the critical index for the correlation length are obtained for both the site and bond problems in the square and simple-cubic lattices.

In recent years, there has been a considerable interest in quantum percolation problems,[1-5] where a crossover between quantum and classical localization will be observed. Quantum percolation problems are usually formulated in terms of a tight-binding one-electron Hamiltonian on a regular lattice[2]

$$H=\sum_n |n\rangle \epsilon_n \langle n| + \sum_{n\neq m} |n\rangle v_{nm}\langle m| \ , \tag{1}$$

where the transfer energy v_{nm} is assumed, for simplicity, to be zero for pairs other than nearest neighbors.[6] As in the classical case, we can define the site and bond processes in quantum percolation: the site process is characterized by constant transfer energy $v_{nm}=1$ and random site energies obeying the probability distribution

$$P(\epsilon_n)=x\delta(\epsilon_n)+(1-x)\delta(\epsilon_n-\infty) \ , \tag{2}$$

and the bond process is characterized by constant site energy $\epsilon_n=0$ and random transfer energy obeying the probability distribution

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

The main concern in quantum percolation problems is to locate the quantum percolation threshold x_q and p_q below which the electron is localized, in the sense described by Anderson,[7] with probability one. The quantum threshold x_q and p_q must not be less than their classical counterparts x_c and p_c.

There have been many estimations of the quantum percolation threshold x_q and p_q for the square and simple-cubic lattices. While some of the earlier works[1,2] based on computer simulation concluded that the difference between the classical and quantum thresholds would be small, recent works showed a significant difference between both thresholds. Raghavan and Mattis,[3] and Raghavan[5] mapped a two- or higher-dimensional system into a one-dimensional chain and studied the fluctuation of the matrix element of the tridiagonal Hamiltonian matrix corresponding to the chain. They obtained the quantum bond percolation threshold $p_q=1.0$, 0.37, 0.23 for the "cubic" lattice in two, three, and four dimensions,[3] respectively, and the quantum site percolation threshold $x_q=0.95$ for the square lattice (with some ambiguity), and 0.48 for the simple-cubic lattice.[5] Shapir, Aharony, and Harris[4] used an averaged susceptibility, a generalization of the inverse participation ratio, as a criterion for percolation and located the critical point by using the Padé approximation. They obtained $p_q=1.0$ and 0.323 for the square and simple-cubic lattices, though these values depend on the order of the Padé approximant. The participation ratio has also been used to locate the threshold by computer simulation,[8-10] but the large fluctuation of the participation ratio makes the estimation less reliable. The quantum percolation in the Bethe lattice has also been studied.[9,11,12]

The purpose of the present paper is to study the quantum percolation process on the basis of the real-space renormalization-group technique and to estimate the percolation threshold for both site and bond processes in the square and simple-cubic lattices from a different point of view. To this end we employ a homomorphic cell renormalization depicted in Fig. 1(a) which has been used in classical percolation problems.[13-15] These cells constitute the sites and bonds in the renormalized lattice which retains the symmetry of the original lattice. We define a site (or bond) occupation probability x' (p') of the renormalized lattice in terms of the original occupation probability x (p)

$$x'=R_S(x) \ , \tag{4a}$$

$$p'=R_B(p) \ , \tag{4b}$$

so that the iteration functions $R_S(x)$ and $R_B(p)$ contain all the essential information of the percolation process. Noting the symmetry of the underlying lattice, we determine x' (p') in such a way that the cell is considered to be occupied if and only if an electron can get across the cell in one direction. Thus, we use the Kadanoff cell shown in Fig. 1(b) in order to choose the form $R_S(x)$ and $R_B(p)$.[13-15]

Now, the transformation $R_S(x)$ and $R_B(p)$ can be written

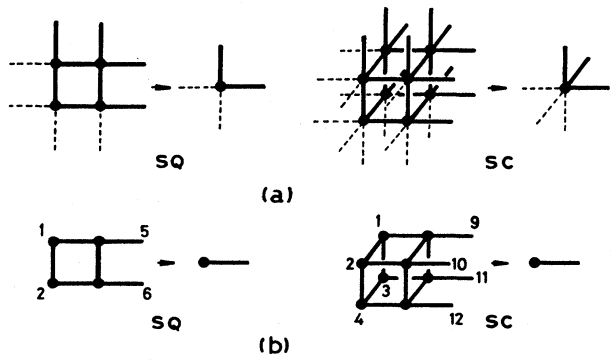

FIG. 1. (a) A homomorphic cell renormalization in the square and simple-cubic lattices. (b) A cell used in the determination of the iteration functions $R_S(x)$ and $R_B(p)$.

in general as

$$R_S(x)=\sum_{n=0}^{N_s}\sum_{i=1}^{{}_{N_s}C_n} S_n(i)x^{N_s-n}(1-x)^n \ , \tag{5a}$$

$$R_B(p)=\sum_{m=0}^{N_B}\sum_{j=1}^{{}_{N_B}C_m} B_m(j)p^{N_B-m}(1-p)^m \ , \tag{5b}$$

where N_S and N_B are the number of sites and bonds, respectively, in the Kadanoff cell. The summations $\sum_i$ in Eq. (5a) and $\sum_j$ in Eq. (5b) go up to ${}_{N_S}C_n$ and ${}_{N_B}C_m$, respectively, to count all possible configurations of "unoccupied site ($\epsilon_n=\infty$)" or "broken bond ($v_{nm}=0$)" in the Kadanoff cell. The coefficients $S_n(i)$ and $B_m(j)$ of a particular configuration (denoted by i and j) can be called the wetting probability of the configuration and represent the ability of the cell configuration in opening a channel for the percolating object from one edge of the cell to the opposite edge. For the classical percolation, the wetting probabilities $S_n(i)$ and $B_m(j)$ are set to unity whenever a channel of occupied site or unbroken bonds connects both edges and zero otherwise.[13–15] When the cell transformation Fig. 1(b) for the simple-cubic lattice is used, for example, $R_S(x)$ for the classical site problem in the simple-cubic lattice [three dimensional (3D)] reads as[15]

$$R_S^{C,3D}(x)=x^8+8x^7(1-x)+28x^6(1-x)^2+56x^5(1-x)^3 +54x^4(1-x)^4+24x^3(1-x)^5+4x^2(1-x)^6 \ . \tag{6}$$

For the quantum percolation, we define the wetting probability as follows: for a given configuration, we first calculate the probability P_α of a particular site α on one edge of the cell [$\alpha=1,2$ for the square lattice and $\alpha=1,2,3,4$ for the simple-cubic lattice in Fig. 1(b)] that an electron left site α at time $t=0$ reaches any sites on the opposite edge after infinite time. The wetting probability of the particular configuration is identified as the averaged probability P_α over all sites in the initial edge, normalized by that of the configuration where all sites are occupied (or all bonds are unbroken). The probability P_α is given by

$$P_\alpha=\sum_\beta P_{\alpha\beta} =\sum_\beta \lim_{t\to\infty} |\langle\beta|e^{-i\tilde{H}t/\hbar}|\alpha\rangle|^2 \ , \tag{7}$$

where $\tilde{H}$ is the Hamiltonian of the Kadanoff cell of the particular configuration and the summation $\sum_\beta$ is taken over all sites in the opposite edge [$\beta=5,6$ for the square lattice and $\beta=9,10,11,12$ for the simple-cubic lattice in Fig. 1(b)]. We can easily show that

$$P_{\alpha\beta}=\sum_\mu |\langle\beta|\mu\rangle\langle\mu|\alpha\rangle|^2 + \sum_{\substack{\mu\neq\nu\\ E_\mu=E_\nu}} \langle\mu|\alpha\rangle\langle\alpha|\nu\rangle\langle\beta|\mu\rangle\langle\nu|\beta\rangle \ . \tag{8}$$

Here, $|\mu\rangle$ and E_μ are the eigenstate and eigenvalue of $\tilde{H}$

$$\tilde{H}|\mu\rangle=E_\mu|\mu\rangle \ . \tag{9}$$

For the quantum site percolation in the simple-cubic lattice, we generated $2^8=256$ configurations of occupied sites and diagonalized the corresponding cell Hamiltonian to obtain the wetting probability through Eq. (8). The renormalization transformation becomes

$$R_S^{Q,3D}(x)=x^8+7.5349x^7(1-x)+21.8365x^6(1-x)^2 +35.8578x^5(1-x)^3+27.2397x^4(1-x)^4 +10.2914x^3(1-x)^5+1.4702x^2(1-x)^6 \ . \tag{10}$$

As usual, the unstable fixed point x^* of the recurrence equation $x'=R_S(x)$ determines the critical percolation probability. We found $x^*\equiv x_c=0.282$ for the classical process[15] and $x^*\equiv x_q=0.701$ for the quantum process. We can also determine the critical index ν for the correlation length by calculating[13]

$$\nu=\ln 2/\ln\lambda \ , \tag{11}$$

where

$$\lambda=\left.\frac{dR_S(x)}{dx}\right|_{x=x^*} \ . \tag{12}$$

We found the index to be $\nu_c=1.23$ for the classical case[15] and $\nu_q=2.28$ for the quantum case.

We also studied the site percolation in the square lattice and the bond percolation in the square and simple-cubic lattices. For each of these three cases, we examined $2^4=16$ configurations, $2^6=64$ configurations, and $2^{16}=65\,536$ configurations to obtain the iteration function. The iteration function for the quantum processes was found to be

$$R_S^{Q,2D}(x)=x^4+3.2818x^3(1-x)+1.3127x^2(1-x)^2$$

for the site problem in the square lattice, and

$$R_B^{Q,2D}(p)=p^6+5.7845p^5(1-p)+9.6274p^4(1-p)^2 +6.0088p^3(1-p)^3+1.3127p^2(1-p)^4$$

for the bond problem in the square lattice and

$$R_B^{Q,3D}(p)=\sum_{n=0}^{14} a_n p^{16-n}(1-p)^n$$

with $a_0=1$, $a_1=16.4955$, $a_2=119.6777$, $a_3=529.1672$, $a_4=1590.563$, $a_5=3482.256$, $a_6=5612.857$, $a_7=6712.185$, $a_8=5956.260$, $a_9=3928.327$, $a_{10}=1907.513$, $a_{11}=662.1523$, $a_{12}=155.8492$, $a_{13}=22.2817$, $a_{14}=1.4702$ for the bond problem in the simple-cubic lattice. Table I summarizes the percolation threshold and the critical index of the correlation length for both the classical and quantum percolation determined by the present method together with values for the classical problem known in the literature.

As has been shown by Reynolds, Klein, and Stanley[13] and Stanley,[14] the cell renormalization employed here works quite well for both the site and bond processes in classical percolation. Therefore, we expect that the quantum percolation threshold obtained here will not differ much from the exact threshold, though we may have to take the large cell limit to obtain more accurate estimation for the percolation threshold and the critical index[20] which is being pursued. It is interesting to note that in the present theory the ratio between the classical and quantum percolation threshold is almost a dimensional invariant; in two dimensions, $x_q/x_c=1.40$ for the site problem and $p_q/p_c=1.53$ for the bond problem, and in three dimensions, $x_q/x_c=2.49$ for the site problem and $p_q/p_c=2.61$ for the bond problem.

Our results do not agree with any of the previous estimations. In particular, it is believed that electrons in two-

TABLE I. Percolation threshold and critical index for correlation length obtained by the homomorphic cell renormalization method. The numbers in ( ) are values for the classical percolation known in the literature (Refs. 16–19).

		Percolation threshold		Critical index	
		Classical	Quantum	Classical	Quantum
Square	Site	0.618 (Ref. 14) (0.593)	0.867	1.64 ($\frac{4}{3}$)	3.35
	Bond	0.500 (Ref. 13) (0.500)	0.765	1.43 ($\frac{4}{3}$)	1.89
Simple cubic	Site	0.282 (Ref. 15) (0.311)	0.701	1.23 (0.88)	2.28
	Bond	0.209 (Ref. 13) (0.249)	0.545	1.03 (0.88)	1.31

dimensional systems are localized except when disorder is absent.[21,22] Thus, the percolation threshold in two dimensions is supposed to be unity, and our results $x_q = 0.765$ for the bond problem and $p_q = 0.867$ for the site problem seem to contradict with the foregoing conclusion drawn for Anderson's localization problem in two dimensions on the basis of the scaling property of conductance. On the other hand, it has been conjectured for hopping conduction that a percolation may occur even when the diffusion constant is zero.[23] We need further studies to clarify the contradiction.

Finally, we expect to observe three regimes of the electronic properties in the quantum percolation model: when $x < x_c$ for the site process (or $p < p_c$ for the bond process), all electrons are confined in small clusters where each cluster is a set of occupied sites mutually connected by unbroken bonds. Since Hamiltonian (1) does not allow tunneling of electrons between two isolated clusters, electrons are considered to be localized in the classical sense as well as in the quantum sense. When $x_c < x < x_q$ ($p_c < p < p_q$), there is an infinitely extended channel, but electrons cannot spread infinitely from their initial position. We may call this the quantum localization regime. When $x > x_q$ ($p > p_q$) an electron has a finite probability that it can travel infinitely far from its initial location. When we change the occupation probability x (p) continuously from zero to one, we will observe a crossover from classical to quantum localization and to the extended regime. By multiplying the filling factor of the simple-cubic lattice to the percolation threshold,[24] we can estimate the crossover volume fraction which is found to be 16% for the classical transition and 36% for the quantum transition. Some experiments in metal-insulator composite systems[25,26] showed that crossovers between different conduction regimes occur at about 20%–24% and 30%–38% of volume fraction of the metallic component. The quantum percolation picture will give an account for the crossovers, and a detailed comparison is under investigation.

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