Large-cell Monte Carlo renormalisation group for quantum percolation

1987 J. Phys. A: Math. Gen. 20 L1027

(http://iopscience.iop.org/0305-4470/20/15/017)

J. Phys. A: Math. Gen. **20** (1987) L1027-L1030. Printed in the UK

LETTER TO THE EDITOR

Large-cell Monte Carlo renormalisation group for quantum percolation

K C Chang† and T Odagaki

Department of Physics, Brandeis University, Waltham, Massachusetts 02254, USA

Received 21 July 1987

Abstract. With the use of a large-cell Monte Carlo renormalisation group method, the quantum percolation threshold is determined to be 0.42 for the site problem and 0.30 for the bond problem in a simple cubic lattice.

Quantum percolation processes have been studied extensively during the past ten years. The main focus of the research has been to locate the quantum percolation threshold. The estimations obtained so far, however, are very scattered and a reliable determination of the threshold has long been awaited. For small systems whose linear dimension is shorter than the localisation length, the threshold for the quantum and classical processes are the same [1]. However, estimations for larger systems indicate a significant difference in the threshold for the quantum and classical percolations [2, 3]. Moreover, recent researches suggested that the critical probability depends on the magnetic field [3] and on the strength of tunnelling [4], and thus a more accurate determination of the threshold becomes very important.

In this letter we present a large-cell Monte Carlo renormalisation group analysis for the quantum site and bond percolations in a simple cubic lattice. The threshold is estimated to be 0.30 for the bond process and 0.42 for the site process, and the critical exponent of the correlation length to be 2.1 for both site and bond problems. We apply the same method to a square lattice. The result for the square lattice is not conclusive. It is safe to say for the square lattice that the threshold is above 0.94 and the correlation length critical exponent is about 2.27.

The quantum percolation process has been formulated by the tight-binding Hamiltonian [1]

$$H = \sum_i |i\rangle \varepsilon_i \langle i| + \sum_{(i,j)=\mathrm{nn}} |i\rangle t_{ij} \langle j| \tag{1}$$

where $\{|i\rangle\}$ is a set of localised orthonormal bases. In the site process the site energy ε_i is assumed to obey the distribution

$$P(\varepsilon_i) = x\delta(\varepsilon_i) + (1-x)\delta(\varepsilon_i - \varepsilon_B) \tag{2}$$

with $\varepsilon_B = \infty$, and $t_{ij} = t$ is a constant. In the bond process the site energies take a constant value (set to zero) and the nearest-neighbour transfer energy t_{ij} obeys the distribution

$$P(t_{ij}) = p\delta(t_{ij} - t) + (1-p)\delta(t_{ij} - t_B) \tag{3}$$

with $t_B = 0$. Sites with infinite site energy and bonds with zero transfer energy represent

†Present address: World Scientific Publishing Co Pte Ltd, Farrer Road, PO Box 128, Singapore 9128.

0305-4470/87/151027+04$02.50

blocks for the motion of a quantum particle governed by the Schrödinger equation with Hamiltonian (1). The percolation threshold is denoted by x_q and p_q for site and bond processes, respectively.

The classical percolation problems have also been formulated as dynamic processes described by a random walk equation in place of the Schrödinger equation [5].

It might be natural to assume the quantum percolation is a special case of the Anderson's localisation problem [6]. In this context, the quantum percolation is a limiting case of a bimodal distribution for the site energy and for (the logarithm of) the transfer energy. The randomness of the bimodal distribution is greatest at 50% of the concentration, and thus one would expect the states to be more localised at this concentration. However, the percolation threshold is believed to be less than 50% in three dimensions [2, 3] and states at 50% are supposed to be more extended than the states near the threshold. Furthermore, one might measure the randomness of a distribution by its second moment. The second moment of the distribution in quantum percolation (for bond problems the second moment of $\log|t_{ij}|$ is used [7]) is infinity and one might expect that all the states must be localised in *any* dimensions except for the pure system [8]. This expectation is totally inconsistent with the observation that there is a percolation transition in three and higher dimensions [1-4]. It is interesting to note that the usual parameter W/t (the ratio of the width of a flat distribution of the site energy to the transfer energy) in Anderson's problem with diagonal disorder also determines the probability that the site energy of two sites differs by less than t. (More precisely, it is $(2-t/W)t/W$.) If we let these sites be connected, then we can estimate the critical value for the Anderson problem by equating this probability to the critical quantum percolation probability. Therefore it is tempting to consider Anderson's problem be a generalised quantum percolation problem.

Now we follow the renormalisation group method developed by us [9] with larger cell size (see figure 1). The estimation is supposed to become more accurate for larger cell sizes. The renormalised occupation probability p' for the bond process (x' for the site process) is determined by the probability that a particle attached to one of the sites on the left edge at $t=0$ appears on the right edge and by a normalisation factor which makes $p=1$ be one of the stable fixed points of the transformation. That is,

$$p' = A\left\langle \frac{1}{b^{d-1}} \sum_{\alpha} \sum_{\beta} P_{\alpha\beta} \right\rangle \equiv R(p) \tag{4}$$

where

$$P_{\alpha\beta} = \lim_{t\to\infty} |\langle \beta | \, \mathrm{e}^{\mathrm{i}Ht/\hbar} | \alpha \rangle|^2 \tag{5}$$

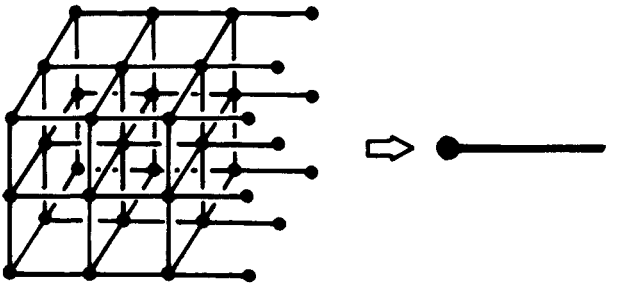

Figure 1. A cell used in the determination of the renormalisation function $R(p)$. This cell corresponds to $b=3$.

is the probability that a particle leaving site α (on the left edge) at time $t=0$ is at site β (on the right edge) at $t=\infty$ for a given configuration, b is the linear dimension of the cell, A is the normalisation factor and $\langle \ldots \rangle$ denotes an ensemble average. In our previous paper [9] the renormalisation function $R(p)$ was calculated exactly for $b=2$ by generating all the configurations and carrying out the ensemble average rigorously. For larger cell sizes, however, it is not practical to generate all of the configurations. Instead, we use a Monte Carlo method to determine the renormalisation function. For a fixed p, we generate many configurations of the cell of linear dimension b. For each configuration we calculate the probability $P_{\alpha\beta}$ and carry out the average in (4) to obtain $R(p)$. Then we plot $R(p)$ against p and determine graphically the unstable fixed point $p^*(b)$ and the slope, $\lambda(b)$ $(\equiv\{dR(p)/dp|_{p=p^*}\})$, of the renormalisation function at the fixed point which in turn is used to find the correlation length critical exponent $\nu(b)$ through $\ln b/\ln \lambda(b)$. We repeat the same process for different values of $b=4$, 6, 8 and 9 taking 50, 30, 5 and 5 samples respectively. The correlation length critical exponent is plotted against $1/b$ and, from the limit of $b=\infty$, ν is estimated to be 2.1. Following the standard procedure [10], the critical probability $p^*(b)$ for the bond problem ($x^*(b)$ for the site problem) is plotted against $b^{-1/\nu}$ which is shown in figure 2 for both site and bond processes in the simple cubic lattice. The limit of this plot at $b^{-1/\nu}=0$ determines the percolation threshold for the infinite cell size. The best guess for the threshold based on the linear extrapolation is

$$x_q = 0.42 \qquad \text{for the site problem} \tag{6}$$

$$p_1 = 0.30 \qquad \text{for the bond problem.} \tag{7}$$

It should be remarked here that the linearity in the plot of $p^*(b)$ against $b^{-1/\nu}$ holds asymptotically as $b^{-1/\nu}$ approaches zero. Therefore, for the range of the cell sizes studied here, it may be possible to exploit extrapolation other than a straight line. For

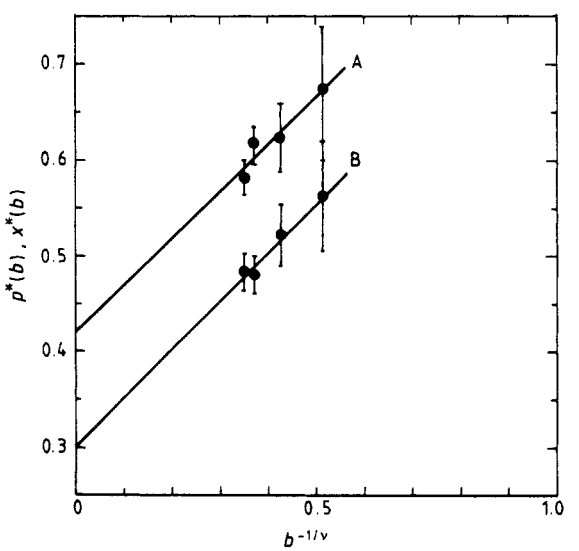

Figure 2. Extrapolation of the sequence of fixed points $p^*(b)$ for the bond problem and $x^*(b)$ for the site problem in the simple cubic lattice obtained from (4) for various cell

example, extrapolation by a parabola yields $x_q = 0.43$ for the site problem. We simply mention here that an error might exist due to the extrapolation and leave the detailed discussion of the effect of the extrapolation as a future study.

We applied the same procesure to the square lattice with $b = 4, 8, 15, 20, 25$ with sample number up to 100. Although the fluctuation of the data is large, $p^*(b)$ appears to increase as the cell size increases, in clear contrast to the plot shown in figure 2 for three dimensions. In view of the large fluctuation, it is safe to say that $\nu \simeq 2.27$, and both p_q and $x_q \geqslant 0.94$.

The present estimation of the critical quantum percolation probability agrees with some of the previous estimations [2-3]. The quantum threshold for site and bond processes are 35% and 21% larger than their classical counterparts, respectively. This implies that three possible conduction regimes exist in percolating systems consisting of a metal and a non-metal. Above the quantum threshold the conduction is governed by the quantum mechanical dynamics and the conductivity is determined by the correlation length, i.e. the conductivity is expected to show a dependence on the occupation probability as $(x - x_q)^{\nu}$ ($\nu = 2.1$ in our estimation) [11]. Below the quantum threshold, a carrier is supposed to be localised and it is not possible to produce conduction alone. However, conduction can take place via phonon assisted hopping. The classical percolation threshold plays a role since below the classical threshold intercluster hopping determines the conductivity and above the classical threshold intracluster hopping within an infinite cluster will give a dominant contribution to the conductivity. Therefore one can expect to observe three conduction regimes in percolating systems. In fact Epstein *et al* [12] observed three conduction regimes in Hg-Xe mixtures. Moreover, in the metallic region the conductivity showed a power law behaviour $(v - v_q)^{2.15}$, v being the volume fraction of Hg and v_q the upper critical volume fraction. The exponent coincides with our estimation. It will be possible to explain two other conduction regimes in Hg-Xe systems from the point of view of hopping conduction, which will be studied in the future.

This work was supported in part by a grant from Research Corporation.

References

[1] Odagaki T, Ogita N and Matsuda H 1980 *J. Phys. C: Solid State Phys.* **13** 189
[2] Shapir Y, Aharony A and Harris A B 1982 *Phys. Rev. Lett.* **49** 486
Evangelou S N 1983 *Phys. Rev.* B **27** 1397
Raghavan R and Mattis D C 1981 *Phys. Rev.* B **23** 4791
Raghavan R 1984 *Phys. Rev.* B **29** 748
Root L and Skinner J L 1986 *Phys. Rev.* B **33** 7738
[3] Meir Y, Aharony A and Harris A B 1986 *Phys. Rev. Lett.* **56** 976
[4] Chang K C and Odagaki T 1987 *Phys. Rev.* B **35** 2598
[5] Odagaki T 1986 *Transport and Relaxation in Random Materials* ed J Klafter, R J Rubin and M F Shlesinger (Singapore: World Scientific) p 278
[6] Anderson P W 1958 *Phys. Rev.* **109** 1492
[7] Odagaki T 1980 *Solid State Commun.* **33** 861
[8] Abraham E, Anderson P W, Licciardello D C and Ramakrishnan T V 1979 *Phys. Rev. Lett.* **42** 673
[9] Odagaki T and Chang K C 1984 *Phys. Rev.* B **30** 1612
[10] Reynolds P J, Stanley H E and Klein W 1978 *J. Phys. A: Math. Gen.* **11** L199; 1980 *Phys. Rev.* B **21** 1223
Eschbach P D, Stauffer D and Herrmann H J 1981 *Phys. Rev.* B **23** 422
[11] Shapiro B 1983 *Percolation Structures and Processes* (*Annals of the Israel Physical Society* **5**) ed G Deutscher, R Zallen and J Adler (Bristol: Adam Hilger) p 367
[12] Epstein K, Goldman A M and Kadin A M 1983 *Phys. Rev.* B **27** 6685