Three-dimensional quantum percolation studied by level statistics

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Abstract. We study the metal-insulator transition on a three dimensional quantum percolation model by analyzing energy level statistics. The quantum percolation threshold \( p_q \), which is larger than the classical percolation threshold \( p_c \), becomes smaller when the time reversal symmetry (TRS) is broken, i.e. \( p_q \) (with TRS) > \( p_q \) (without TRS) > \( p_c \). It is shown that critical exponents are consistent with the result of the Anderson transition, suggesting that the quantum percolation problem can be classified into the same universality classes of the Anderson transition. The shape of level statistics at the critical point is also reported.

Keywords: quantum percolation, Anderson transition, universality

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1 Introduction

Due to its simple but non-trivial nature, percolation problems have been attracting a lot of attention [1]. Especially interesting is its application to the transport properties in three-dimensional disordered solids. However, at low temperature, the quantum interference effects should be seriously taken into account and the classical percolation picture is insufficient. Thus the study of the quantum percolation problem becomes a very important subject.

It is well known that disordered systems show the Anderson metal-insulator transition. This is classified into three universality classes (orthogonal, unitary, and symplectic universality classes) by time-reversal and spin-rotation symmetry. This conjecture is well confirmed for the Anderson tight binding model [2]. Then it is natural to ask whether the quantum percolation problem can be also classified into the same universality classes of the Anderson transition. If yes, the critical exponent \( \nu \) for the divergence of the localization length in the quantum percolation model is the same as in the Anderson model, namely, \( \nu = 1.57 \pm 0.02 \) in the presence of the time reversal symmetry (TRS) [2, 3], and \( \nu = 1.43 \pm 0.02 \) in the absence of it [3]. However, the estimates of \( \nu \) in the quantum percolation problem reported so far are at variance. For example, renormalization group analyses of the quantum percolation problem give \( \nu = 2.1 \pm 0.1 \) [4], \( \nu = 1.9 \pm 0.5 \) [5], and \( \nu = 1.86 \pm 0.12 \) [6], well above the value in the Anderson model. From the Thouless number analysis, it is estimated to be \( \nu = 1.95 \pm 0.12 \) [7, 8], again larger than in the Anderson model. On the other hand, the transfer matrix method for the network model gives \( \nu = 0.75 \pm 0.1 \) [9], and the
analytic estimate of the transmission coefficient gives $\nu = 0.38 \pm 0.07$, significantly smaller than in the Anderson model. Recently, using the finite size scaling behavior of level statistics [12], Berkovits and Avishai estimated $\nu$ to be $1.35 \pm 0.1$, not far from the value of the Anderson model. Inspired by their work, we perform extensive numerical study of the level statistics on the percolation cluster. We also study the effect of breaking of TRS.

2 Model and method

To describe the three dimensional (3D) quantum bond percolation model, we consider the following tight-binding Hamiltonian

$$H = \sum_{\langle ij \rangle} (t_{ij} a_i^\dagger a_j + H.c)$$

(1)

where $\langle ij \rangle$ denotes nearest neighbors. The transfer energy is defined as

$$t_{ij} = \begin{cases} \exp(i\theta_{ij}) & \text{(for connected bond)} \\ 0 & \text{(for disconnected bond)} \end{cases}$$

(2)

Bonds are randomly connected with probabilities $p$. $\theta_{ij}$ is the Peierls phase due to magnetic field. When all the Peierls phases are set to 0, the Hamiltonian is time reversal symmetric, and we call it TRS model. When the phases are not vanishing, the Hamiltonian is generally not time reversal symmetric. We set $-\pi < \theta_{ij} < \pi$ randomly, and call this situation non-TRS model hereafter. The underlying lattice is a three-dimensional cube of length $L$ with periodic boundary conditions. For each realization of bond structure, we first find maximally percolating cluster and then we diagonalize it by Lanczos method. In order to gain good statistics, more than $10^6$ eigenvalues are calculated, so the number of realizations of random bond configuration are $N = 580, 300, 175$ and $110$ for sample sizes $L^3 = 12^3, 15^3, 18^3$ and $21^3$. We take levels in the region $0.2 < |E| < 0.8$ where density of states is rather smooth [13].

Then the distribution function $P(s)$ of adjacent level spacings $s$ is calculated. In the limit of large system size $L \to \infty$, the level spacing distribution $P(s)$ is expected to be described by Poisson distribution $P(s) = \exp(-s)$ in the insulator region. In the metallic regime, $P(s)$ is well described by the Wigner surmise, $P(s) \propto s^\beta \exp(-A_\beta s^2)$ ($\beta = 1$ in the presence of TRS and $\beta = 2$, otherwise).

In order to obtain the critical value of the probability $p_\xi$ and critical exponent $\nu$, we define $I(s)$ and $\Lambda(p, L)$ as

$$\Lambda(p, L) = \frac{\int_0^{s_0} I(s) ds - \int_0^{s_0} I_p(s) ds}{\int_0^{s_0} I_w(s) ds - \int_0^{s_0} I_p(s) ds}, \quad I(s) = \int_0^s P(s') ds'$$

(3)

which characterizes the transition from Poisson to Wigner. $s_0$ is set to 1.2. Noting that $\xi(p)$ diverges as

$$\xi(p) \sim |p - p_\xi|^{-\nu},$$

(4)
Fig. 1 Level spacing distribution for TRS (a) and non-TRS (b) models at the critical point. The system size is $L = 21$ for example, but the form is almost independent of $L$.

near the critical probability $p_q$, $\Lambda(p, L)$ is expected to behave as

$$\Lambda(p, L) = f[L/\xi(p)] = a_0 + a_1[L(p - p_q)]^{1/\nu} + a_2[L(p - p_q)]^{2/\nu} + \cdots.$$  \hspace{1cm} (5)

Fitting the data to this expression, we estimate $p_q$ and $\nu$.

3 Result

The results are summarized in Table I. When magnetic fields are applied, the critical point $p_q$ of non-TRS model becomes smaller than that in the presence TRS, suggesting that this transition has a nature of the Anderson transition. Note that $p_q$ is much larger than the classical bond percolation threshold $p_c \approx 0.249$. This is why taking all energy levels including small clusters [13] and taking only those in the largest cluster make small difference [14, 15]. Both TRS and non-TRS models show $\nu$ consistent with the value of the Anderson transition [15].

We then compare the shape of level statistics at the critical point $p_q$ (Fig. 1). It is clearly seen that the critical level statistics is sensitive to the breaking of TRS.

In the large $s$ region, the level statistics is described by the sub-Poisson form, $\propto \exp(-\kappa s)$ (Fig. 2). In the Anderson model, $\kappa = 1.9 \pm 0.1$ for the orthogonal symmetry [16] and 1.87 for unitary symmetry [17]. In the present quantum percolation model, $\kappa = 1.77 \pm 0.10$ in the presence of TRS, and for non-TRS model $\kappa = 1.87 \pm 0.03$.

The overall form of the critical level spacing distribution deviates from those in the Anderson model with periodic boundary condition (b.c.) and the fixed b.c. [16]. Detailed will be reported elsewhere.

References
Fig. 2  Semi-log scale level spacing distribution for TRS(a) and non-TRS model(b). We fit the curve to $C\exp(-\kappa s)$ with $\kappa = 1.77$ for TRS model and $\kappa = 1.87$ for non-TRS model.

$\log p(s)$

$s$

(a)

(b)

Table 1  The critical point $p_0$ and the critical exponent $\nu$ with their standard deviations.

The values of the TRS model and the non-TRS model are only for percolating cluster, while TRS (all) is obtained from all energy levels. TRS (all, BA) is the result reported in ref. [13].

| system          | size         | $p_0$       | $\nu$       |
|-----------------|--------------|-------------|-------------|
| TRS (all,BA)    | $L = 7,9,11,13,15$ | $0.33 \pm .01$ | $1.35 \pm .10$ |
| TRS (all)       | $L = 12,15,18,21$ | $0.321 \pm .001$ | $1.45 \pm .07$ |
| TRS             | $L = 12,15,18,21$ | $0.324 \pm .001$ | $1.42 \pm .07$ |
| non-TRS         | $L = 15,18,21$  | $0.324 \pm .001$ | $1.45 \pm .11$ |
| non-TRS         | $L = 12,15,18,21$ | $0.309 \pm .001$ | $1.13 \pm .05$ |
| non-TRS         | $L = 15,18,21$  | $0.308 \pm .001$ | $1.25 \pm .08$ |

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