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Disorder-induced quantum bond percolation

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Abstract
We investigate the effects of off-diagonal disorder on localization properties in quantum bond percolation networks on cubic lattices, motivated by the finding that the off-diagonal disorder does not always enhance the quantum localization of wavefunctions. We numerically construct a diagram of the 'percolation threshold', distinguishing extended states from localized states as a function of two degrees of disorder, by using the level statistics and finite-size scaling. The percolation threshold increases in a characteristic way on increasing the disorder in the connected bonds, while it gradually decreases on increasing the disorder in the disconnected bonds. Furthermore, the exchange of connected and disconnected bonds induced by the disorder causes a dramatic change of the percolation threshold.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The problem of quantum localization of wavefunctions in disordered systems has received intensive attention since the pioneering work by Anderson [1–7]. The Anderson model for a disordered system is typically described using the tight-binding one-electron Hamiltonian,

$$H = \sum_{n} \varepsilon_n |n\rangle\langle n| + \sum_{m,n(m\neq n)} t_{m,n} |m\rangle\langle n|, \qquad (1)$$

where $|m\rangle$ (or $|n\rangle$) indicates the orthonormalized atomic orbital at site m (or n), ε_n denotes the orbital energy and $t_{m,n}$ denotes the energy of transfer between the sites m and n.

Quantum percolation, defined as the quantum version of the classical percolation by Broadbent and Hammersley [8, 9], is described as a special case of the disordered system in which ε_n randomly takes the values 0 and ∞ while $t_{m,n} = t$ is a constant in the case of site percolation, and $t_{m,n}$ randomly takes the values t and 0 while $\varepsilon_n = 0$ in the case of bond percolation. Quantum percolation scenarios have been discussed in efforts to obtain an understanding of unusual electronic transport properties such as the colossal magnetic resistance in perovskite manganite films [10, 11] and minimal conductivity in graphene [12]. Furthermore, it has been debated whether the localization–delocalization transition occurs even in two-dimensional percolation networks [13, 14].

Another topic of interest is the effect of diagonal and off-diagonal disorder on the quantum percolation threshold p_q which distinguishes extended states from localized states. In the case of site percolation, it has been observed that p_q increases on introducing disorder into site energies because the disorder enhances the localization [15–17]. However, we have not known much about the case of bond percolation [17, 18]. The effect of off-diagonal disorder on localization is not simple even in ordinary disordered systems. Previous studies reported that wavefunctions around the band center are not localized irrespective of the strength of the disorder, because the off-diagonal disorder both enhances and suppresses the localization of eigenstates [19, 20]. Therefore, it is worth studying the effect of off-diagonal disorder on the localization–delocalization transition, starting from the bond percolation Hamiltonian.

In this paper, we numerically examine disordered quantum bond percolation networks and derive a diagram of the percolation threshold describing the localization–delocalization transition as a function of two types of disorder

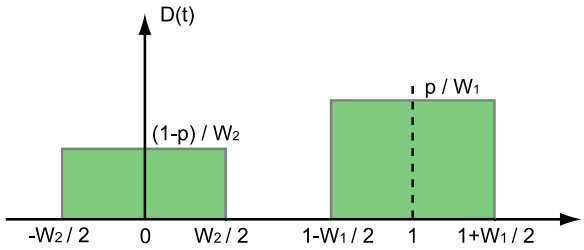

Figure 1. Schematic illustration of $D(t)$ described by equation (2).

for connected and disconnected bonds. We find some novel effects of off-diagonal disorder on the quantum percolation threshold, in contrast with the diagonal disorder case: (i) the quantum percolation threshold p_q is only weakly influenced by weak and strong disorders of connected bonds; (ii) p_q drastically changes for medium disorder of connected bonds; (iii) disorder of disconnected bonds suppresses p_q.

In section 2, we introduce disordered quantum bond percolation networks and show the level spacing distribution $P(s)$ of the system. The diagram is shown in section 3 and the final section is devoted to a summary and discussion.

2. Level spacing distribution in disordered bond percolation networks

The problem of off-diagonal disorder in the (nearest-neighbor) bond percolation on a cubic lattice is described by introducing the following independent identical probability distribution for each of the nearest-neighbor transfer energies t:

$$D(t) = p\frac{1}{W_1}\theta\left(\frac{W_1}{2} - |t - t_0|\right) + (1-p)\frac{1}{W_2}\theta\left(\frac{W_2}{2} - |t|\right), \quad (2)$$

where $0 \leqslant p \leqslant 1$ is the probability of a connected bond of strength t_0, θ is the step function taking the values 0 and 1 for negative and positive arguments respectively, and W_1 and W_2 are the widths of the two constituent box distributions of the connected bond and the disconnected bond respectively. We put $t_0 = 1$ in this paper. The distribution function $D(t)$ is visualized in figure 1.

Each sample system is generated on the cubic lattice of linear size L using equation (2) for the nearest-neighbor bond and adopting a cyclic boundary condition. We obtain N $(=L^3)$ eigenvalues by diagonalizing the Hamiltonian of the disordered quantum bond percolation network. A typical distribution of eigenvalues (density of states) is shown in figure 2. The strength of disorder W_1 contributes smoothing of the detailed spiky structure of the density of states, due to the existence of small disconnected clusters, except the one at the band center [21]. The singularity at the band center is sensitive to the strength of the disorder in the disconnected bond, that is W_2. To avoid the singularity at the band center, we focus our attention on a fairly small energy interval $[-0.6, -0.2]$ near the band center, in which the sample-averaged density of states looks almost constant.

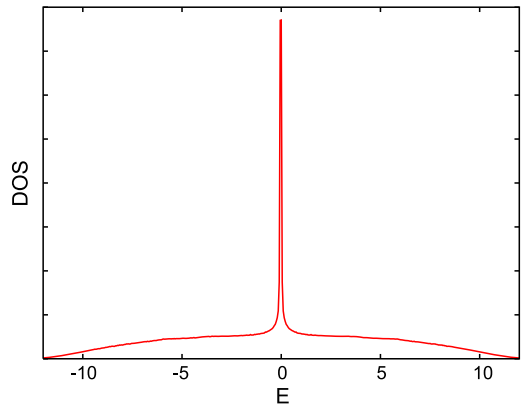

Figure 2. Sample-averaged density of states for the case $p = 0.46$, $W_1 = 10.0$, $W_2 = 0.1$ and $L = 12$.

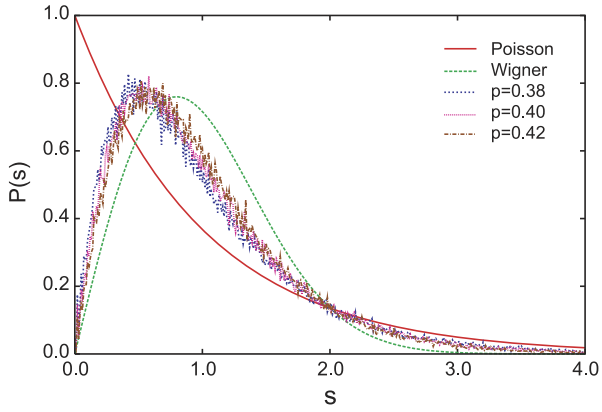

Figure 3. Level spacing distribution $P(s)$ for the case $W_1 = 2.0$ and $W_2 = 0.2$. The Wigner distribution and the Poissonian one are displayed for reference.

It should be noted that the density of states of the disordered bond percolation network is smoother than that of the conventional bond percolation network over a wide range of p. This is because the off-diagonal disorder of disconnected bonds suppresses the classical percolation threshold p_c, so most of the states belong to the percolating cluster even for small p. In this paper, we consider only the region which is at a distance from the classical percolation threshold p_c to avoid seeing the energy levels of small disconnected clusters.

In order to investigate localization properties of electronic states in the system, we examine the level statistics of the energy spectra, which is a powerful tool for finding the localization–delocalization transition in percolation networks [22–24]. The random matrix theory states that the level spacing distribution $P(s)$ is the Wigner distribution for extended states and the Poissonian distribution for localized states [22]. We use a lot of sample systems of the order of roughly 10^3 or 10^4 so that we obtain 10^5 eigenvalues in the energy interval $[-0.6, -0.2]$ to determine the $P(s)$. The unfolding procedure is applied to eliminate the energy dependence of the mean level spacing [25]. The level spacing distribution $P(s)$ for $W_1 = 2.0$ and $W_2 = 0.2$ with varying p is exemplified in figure 3. The change in $P(s)$ from

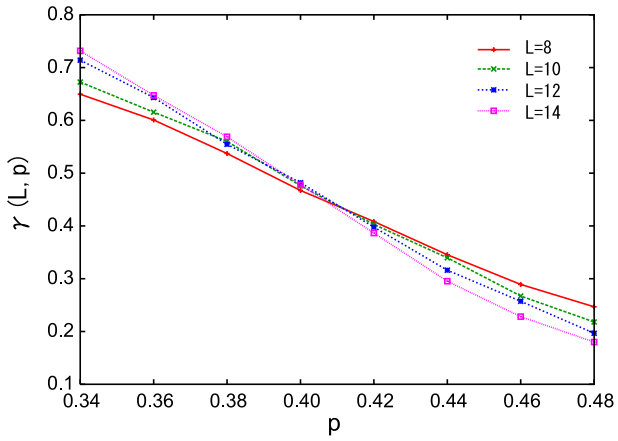

Figure 4. $\gamma(L, p)$ as a function of p for the case $W_1 = 2.0$ and $W_2 = 0.2$. The value of p at size-independent γ gives the percolation threshold p_q.

the Poissonian distribution to the Wigner distribution with increasing p indicates that electronic states become extended for large values of p. Although it is expected that the $P(s)$ for lower p clearly follows the Poissonian distribution, we calculate the $P(s)$ only near the quantum percolation threshold p_q to escape taking into account the energy levels of small disconnected clusters.

3. Localization–delocalization transition in disordered bond percolation networks

We extract information on the localization–delocalization transition from $P(s)$ with varying probability p and system size L, in order to determine the percolation threshold p_q. It is known that the finite-size scaling analysis of the level spacing distribution is useful for finding the critical value of the probability p_q [18]. We evaluate a quantity $\gamma(L, p)$ defined as

$$\gamma(L, p) \equiv \frac{A - A_{\mathrm{W}}}{A_{\mathrm{P}} - A_{\mathrm{W}}}, \tag{3}$$

$$A(L, p) \equiv \int_2^\infty P(s, L, p)\, \mathrm{d}s, \tag{4}$$

where A_{P} and A_{W} are the same integrals for the Poissonian distribution $P_{\mathrm{P}}(s)$ and the Wigner distribution $P_{\mathrm{W}}(s)$, respectively [22]. In figure 4 we show γ as a function of p for the case of $W_1 = 2.0$ and $W_2 = 0.2$, and different system sizes $L = 8$, 10, 12 and 14. It is clearly seen that all curves cross at a single point of p where γ is independent of the system size, namely at the percolation threshold p_q.

Our numerically obtained diagram for $p_q(W_1, W_2)$ is shown in figures 5 and 6. For fairly small ranges of W_1 and W_2, the percolation threshold is insensitive to the strength of disorder W_1 of the originally connected bonds and depends linearly on W_2 for the originally disconnected bonds as shown in figure 5. The off-diagonal disorder around $t_0 = 1$ both enhances and suppresses the multiple-scattering processes through the increasing and decreasing of the rates of transition between orbitals. The two effects seem to cancel to each other

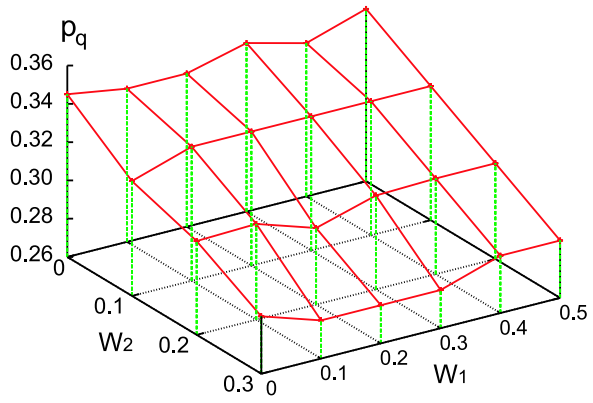

Figure 5. Narrow view of the percolation threshold p_q as a function of W_1 ($\leqslant 0.5$) and W_2 ($\leqslant 0.3$).

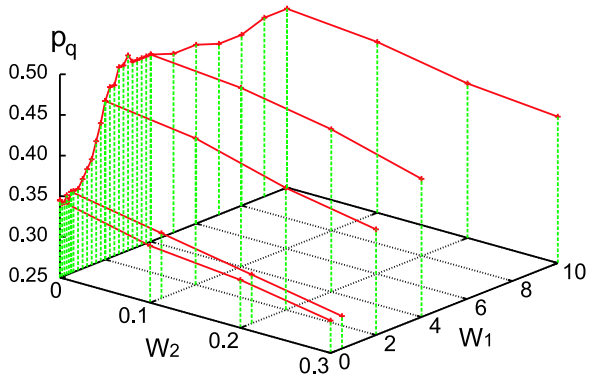

Figure 6. Wide view of the percolation threshold as a function of W_1 and W_2.

and to yield a W_1-independent property for p_q. In contrast to this, the disorder W_2 around the originally disconnected bond enhances the transition because the starting point is perfectly disconnected. This may be understood as the extreme case where $t_0 = 0$. The disorder partially connects the originally disconnected bonds and lowers the percolation threshold of the original network.

Furthermore, another behavior of the percolation threshold is observed when we extend the range of W_1 up to 10.0 as shown in figure 6. The percolation threshold dramatically increases around $W_1 = 2.0$ due to the fact that the originally connected bond begins to become partially disconnected in the region of W_1. On the other hand, we meet again a flat area when the value of W_1 is larger than 3.0. We also examine the case of $W_1 = 20.0$, and have found the same behavior of the percolation threshold. The peculiar behavior of the percolation threshold which is independent of the strength of the disorder W_1 is quite interesting; however, we do not have an explanation for the overview being so flat in the area of larger W_1.

It is also remarkable that the effect of disorder W_2 on the originally disconnected bond always shows the same feature, independent of the value of the strength of disorder W_1 of the originally connected bond. Unfortunately, we could not calculate the $P(s)$ for the strongly disordered regime of W_2 so the phase diagram of the percolation threshold is restricted for W_2.

The strong disorder causes sharper peaks of the density of states and destroys the flatness of the density of states in the energy range $[-0.6, -0.2]$. However, if the behavior of p_q remains linearly dependent of W_2 even for $W_2 > 0.3$, the percolation threshold $p_q(W_1 \leqslant 0.5, W_2)$ is expected to vanish for $W_2 \cong 2.0$, in which region most of the bonds become connected.

4. Summary and discussion

To summarize, we numerically examined the effect of off-diagonal disorder in quantum bond percolation networks on cubic lattices. We calculated a phase diagram for the percolation threshold p_q as a function of two kinds of strengths of disorder, namely that of the disorder on the connected bonds W_1 and that of the disorder on the disconnected bonds W_2, by using the finite-size scaling of the level spacing distribution. We found that the percolation threshold p_q is independent of the strength of disorder W_1 for the ranges $W_1 \leqslant 1.0$ and $W_1 \geqslant 3.0$ and increases dramatically for $1.0 \leqslant W_1 \leqslant 3.0$. The connected bond begins to be disconnected by the disorder W_1 at around 2.0, so the localization of the electronic states is enhanced, and higher p_c is observed. We further found that the percolation threshold linearly decreases with increasing W_2 irrespective of the strength of disorder W_1. Although we could not obtain the p_c for larger W_2 due to singularities of the density of states, it is expected that the percolation threshold will vanish for larger W_2 and that all electronic states will become extended in a strongly disordered regime. Off-diagonal disorder in percolation networks produces a rich phase diagram for the percolation threshold, in contrast with diagonal disorder, because it enhances and suppresses the localization of the electronic states.

Acknowledgments

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References

[1] Anderson P W 1958 *Phys. Rev.* **109** 1492
[2] See a review by Lifshitz I M, Gredeskul S A and Pastur A 1988 *Introduction to the Theory of Disordered Systems* (New York: Wiley)
[3] See a review by Kramer B and Mackinnon A 1993 *Rep. Prog. Phys.* **56** 1469
[4] See a review by Soukoulis C M and Economou E N 1999 *Waves Random Media* **9** 255
[5] Kotani S 1984 *Stochastic Analysis* ed K Ito (Amsterdam: North-Holland) p 225
[6] Ishii K 1973 *Suppl. Prog. Theor. Phys.* **53** 77
[7] Abrahams E, Anderson P W, Licciardello D C and Ramakrishnam T B 1979 *Phys. Rev. Lett.* **42** 673
[8] Broadbent S R and Hammersley J M 1957 *Proc. Camb. Phil. Soc.* **53** 629
[9] See a review by Essam J W 1980 *Rep. Prog. Phys.* **43** 833
[10] Zhang L, Israel C, Biswas A, Green B L and de Lozanne A 2002 *Science* **298** 805
[11] Becker T, Streng C, Luo Y, Moshnyaga V, Damaschke B, Shannon N and Samwer K 2002 *Phys. Rev. Lett.* **89** 237203
[12] Cheianov V V, Fal'ko V I, Altshuler B L and Aleiner I L 2007 *Phys. Rev. Lett.* **99** 176801
[13] Schubert G and Fehske H 2008 *Phys. Rev.* B **77** 245130
[14] Islam M F and Nakanishi H 2008 *Phys. Rev.* E **77** 061109
[15] Soukoulis C M, Economou E N and Grest G S 1987 *Phys. Rev.* B **36** 8649
[16] Soukoulis C M and Grest G S 1991 *Phys. Rev.* B **44** 4685
[17] Soukoulis C M, Li Q and Grest G S 1992 *Phys. Rev.* B **45** 7724
[18] Berkovits B and Avishai Y 1996 *Phys. Rev.* B **53** R16125
[19] Antoniou P D and Economou E N 1977 *Phys. Rev.* B **16** 3768
[20] Cain P, Roemer R A and Schreiber M 1999 *Ann. Phys., Lpz.* **8** 507
[21] Kirkpatrick S and Eggarter T P 1972 *Phys. Rev.* B **6** 3598
[22] Mehta M L 1991 *Random Matrices* (San Diego, CA: Academic)
[23] Shklovskii B I, Shapiro B, Sears B R, Lambrianides P and Shore H B 1993 *Phys. Rev.* B **47** 11487
[24] Kaneko A and Ohtsuki T 1999 *J. Phys. Soc. Japan* **68** 1488
[25] Ono Y, Kuwano H, Slevin K, Ohtsuki T and Havlin S 1993 *J. Phys. Soc. Japan* **62** 2762