Localization-delocalization transitions in a two-dimensional quantum percolation model: von Neumann entropy studies

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In two-dimensional quantum site-percolation square lattice models, the von Neumann entropy is extensively studied numerically. At a certain eigenenergy, the localization-delocalization transition is reflected by the derivative of von Neumann entropy which is maximal at the quantum percolation threshold \( p_q \). The phase diagram of localization-delocalization transitions is deduced in the extrapolation to infinite system sizes. The non-monotonic eigenenergies dependence of \( p_q \) and the lowest value \( p_q \approx 0.665 \) are found. At localized-delocalized transition points, the finite scaling analysis for the von Neumann entropy is performed and it is found the critical exponents \( \nu \) not to be universal. These studies provide a new evidence that the existence of a quantum percolation threshold \( p_q < 1 \) in the two-dimensional quantum percolation problem.

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I. INTRODUCTION

The Anderson model\(^{1,2,3,4}\) and the quantum percolation (QP) model\(^{5,6,7,8}\) are two important theoretical models that are used to study electron localization properties in disordered systems. In the two models, the on-site energy randomness and the geometric randomness are considered, respectively. For the Anderson model, there are extensive studies and definitive results\(^{9,10}\), while for the QP model, there are many open issues even today.

The main concern in QP problems is to locate the QP threshold \( p_q \) (accessible site concentrations by quantum particles) below which the electron is localized with probability one. For the Anderson model and the QP model, there is a consensus on the existence of localization-delocalization transitions (LDTs) in three dimensions (3D)\(^{3,6,7,8}\). For Anderson models, according to the one-parameter scaling theory\(^{11}\), LDTs do not occur at and below two dimensions (2D). However, whether the scaling theory is suitable for the QP model is an open question\(^{12}\) and even whether LDTs exist in 2D QP models at \( p_q < 1 \) is less clear\(^{13}\). Studies such as the scaling work based on numerical calculations of the conductance\(^{12}\) and transfer matrix methods with finite-size scaling analysis\(^{14,15}\) showed no evidence for LDTs. At the same time, there are many studies that claim LDTs exist\(^{14,15,16,17,18}\). However, the values of QP threshold \( p_q \) obtained by different methods are not consistent. For example, for 2D quantum site-percolation square lattice models, Odagaki, et al., obtained \( p_q \approx 0.59 \) by a Green’s function method\(^{14}\). Koslowski and von Niessen gave \( p_q \approx 0.70 \) with the Thouless number based on the Thouless-Edwards-Licciardello method\(^{15}\). Srivastava and Chaturvedi showed \( p_q \approx 0.73 \) with the participation used by the method with equations of motion\(^{16}\). Odagaki and Chang found \( p_q \approx 0.87 \) using a real space renormalization-group method\(^{17}\). Raghavan obtained \( p_q \approx 0.95 \) by mapping a 2D system into a one-dimensional system\(^{18}\). Very recently, Islam and Nakanishi suggested that \( p_q \) depending on particle energies by calculating the transmission coefficient for 2D bond-percolation models\(^{19}\).

In the mean time, metal states or metal-insulator transitions are observed experimentally in a variety of dilute two-dimensional electron and hole systems\(^{20-22}\). At the same time, the unusual transport properties of novel materials\(^{23,24}\), such as metal-insulator transitions happen in perovskite manganite films\(^{25}\) and in granular metals\(^{26}\), and minimal conductivity in undoped graphenes\(^{27}\), may be explained by 2D QP models. Therefore these give additional motivations to study LDTs in 2D QP models.

On the other hand, quantum entanglement, which attracting much attention in quantum information\(^{28}\), has been extensively applied in condensed matter physics\(^{29,30,31,32,33,34}\). For example, quantum entanglement measured by the von Neumann entropy was studied in the extended Hubbard model\(^{35,36}\), in quantum small-world networks\(^{35}\), in two interacting particle systems\(^{36}\), in the extended Harper model\(^{37,38}\), in three dimensional Anderson models\(^{39}\), in the integer quantum Hall system\(^{40}\), and in spin models\(^{33,34}\). It is found that the von Neumann entropy shows singular behaviors at quantum critical points(QCPs). The derivative of von Neumann entropy has very good finite size scaling behaviours close to QCPs even for quite small system sizes\(^{38,33,34}\). Therefore it becomes a powerful method to quantify QCPs in various systems.

In this paper, with the help of the von Neumann entropy we present a detailed numerical study of LDTs in the 2D quantum site-percolation model\(^{1}\). Our studies show that a quantum site-percolation threshold \( p_q < 1 \) exists in the 2D QP problem. In the next section the QP model and the definition of von Neumann entropy are introduced. In Sec. III the numerical results are presented. And we present our conclusions and discussions in Section IV.
II. QUANTUM SITE-PERCOLATION MODEL AND VON NEUMANN ENTROPY

A. Quantum site-percolation model

Let us consider one-electron tight-binding Hamiltonian with diagonal disorder defined on square lattices of sites. The on-site potential $\xi_i$ can be drawn from the bimodal distribution

$$p(\xi_i) = p\delta(\xi_i - \xi_A) + (1-p)\delta(\xi_i - \xi_B).$$

In the limit $\xi_B - \xi_A \to \infty$, the electron moves only on a random assembly of A-lattice points. Without loss of generality we choose $\xi_A = 0$. In the situation the A-site occupation probability is $p$ and the corresponding quantum site-percolation Hamiltonian reads

$$H_{AA} = -t \sum_{\langle ij \rangle \in A} (c_i^\dagger c_j + H.c.),$$

where the summation extends over nearest-neighbor A-sites only.

B. von Neumann entropy

The general definition of entanglement is based on the von Neumann entropy. The generic eigenstate $|\alpha\rangle$ for Hamiltonian $H$ with eigenenergy $\varepsilon_\alpha$ is the superposition

$$|\alpha\rangle = \sum_{i \in A} \psi^\alpha_i |i\rangle = \sum_{i \in A} \psi^\alpha_i c_i^\dagger |0\rangle,$$

where $|0\rangle$ is the vacuum and $\psi^\alpha_i$ is the amplitude of wave function at $i$th site. For an electron in the system, there are two local states at each site, i.e., $|1\rangle$ and $|0\rangle$, corresponding to the state with (without) an electron at the $i$th site, respectively. The local density matrix $\rho_i$ is defined by

$$\rho_i = z_i |1\rangle_i \langle 1| + (1 - z_i) |0\rangle_i \langle 0|,$$

where $z_i = \langle \alpha | c_i^\dagger c_i | \alpha \rangle = |\psi^\alpha_i|^2$ is the local occupation number at $i$th site. Consequently, the corresponding von Neumann entropy related to the $i$th site is

$$E^\alpha_{vi} = -z_i \log_2 z_i - (1 - z_i) \log_2 (1 - z_i).$$

For nonuniform systems, the value of $E^\alpha_{vi}$ depends on the site position $i$. At an eigenstate $\alpha$, we define a site-averaged von Neumann entropy

$$E^\alpha_v = \frac{1}{N} \sum_{i=1}^N E^\alpha_{vi},$$

were $N$ is the number of A-lattice sites. The definition shows that for an extended state that $\psi^\alpha_i = \delta_{i0}$ ($i_0$ is a given site) , $E^\alpha_v = 0$. In the present paper all the values of $E^\alpha_v$ is scaled by $\frac{1}{N} \log_2 N$. From the two examples, we know the scaled $E^\alpha_v$ is near 1 when eigenstates are extended, and near zero when eigenstates are localized. Henceforth, we omit “scaled” for simplicity.

For a random system the site-averaged von Neumann entropy $E^\alpha_v$ should be further averaged over different realizations of disorder. The resulting quantity, the disorder averaged von Neumann entropy denoted by $\langle E^\alpha_v \rangle$ for eigenenergy $\varepsilon_\alpha$, which is defined as

$$\langle E^\alpha_v \rangle = \frac{1}{N} \sum_{i=1}^N E^\alpha_{vi} = \frac{1}{K} \frac{1}{N} \sum_{i=1}^N E^\alpha_{vi},$$

where $\overline{X}$ is denoted as random average, $K$ is the number of disorder realizations. In practice, $\langle E^\alpha_v \rangle$ is the average values over a small window $\Delta$ around an energy value $\varepsilon$, i.e., $\varepsilon_\alpha \in [\varepsilon - \Delta/2, \varepsilon + \Delta/2]$. We ensure that $\Delta$ is sufficiently small, and at the same time there are enough states in the interval $\Delta$. Here $\Delta = 0.04$ is chosen and other $\Delta$ give similar results.

Another quantitative measure that is widely used to characterize localization is the participation ratio(PR).

III. NUMERICAL RESULTS

In numerical calculations, we directly diagonalize the eigenvalue Eq. with the periodic boundary condition and obtain all eigenvalues $\varepsilon_\alpha$ and the corresponding eigenstates $|\alpha\rangle$. Without loss of generality, the hopping integral $t$ is taken as units of energy. From formulas , we can obtain the von Neumann entropy $\langle E^\alpha_v \rangle$. We consider systems of linear size $L = 20, 30, \ldots, 60$ (measured in units of the lattice constant) and having $N = L^2$ A-lattice sites in total. The corresponding number of disorder realizations $K = 2500, 2000, \ldots, 500$, respectively. More realizations give similar results.

Before discussing possible localized-delocalized transitions let us investigate the behavior of the von Neumann entropy $\langle E^\alpha_v \rangle$ at different site occupation probability $p$. The $\langle E^\alpha_v \rangle$ as functions of eigenenergies $\varepsilon_\alpha$ are plotted in Figs. at $L = 20, 40$ and 60 for $p = 0.2, 0.7$ and 0.9, respectively. It shows that at the same $p$, the values of $\langle E^\alpha_v \rangle$ depend on eigenenergies $\varepsilon_\alpha$ and system sizes $L$. 

\[\text{Figure} \quad \text{Caption} \quad \text{Figure} \quad \text{Caption} \quad \text{Figure} \quad \text{Caption} \]
For $p = 0.7$ and $0.9$, the $\langle E^v_\alpha \rangle$ are relatively small for eigenstates near the band edges, while relatively large for eigenstates near the band center except eigenstates very near the band edges. Comparing the values of $\langle E^v_\alpha \rangle$ for the three $p$ at the same $L$, on the whole, all $\langle E^v_\alpha \rangle$ are relatively small for $p = 0.2$ and relatively large for $p = 0.9$. Compared to our results, the PR are also plotted in Fig.1(d) for $L = 60$ at the three $p$. The variations of the PR $\langle \xi_\alpha \rangle$ with respect to $\varepsilon_\alpha$ are similar to that of $\langle E^v_\alpha \rangle$ in Figs.(a)-(c). At the same time, the $\langle E^v_\alpha \rangle$ versus the corresponding $\xi_\alpha$ are plotted in Fig.2. It shows that the $\langle E^v_\alpha \rangle$ increases monotonously with the $\langle \xi_\alpha \rangle$, so the von Neumann entropy can reflect the localization properties of eigenstates in the QP model.

To exactly locate localized-delocalized transition points and the corresponding critical exponents with a finite-size scaling analysis, in the follows, we study the von Neumann entropy $\langle E^v_\alpha \rangle$ changes with the site occupation probability $p$ for different eigenenergies. We found that the general trend for all von Neumann entropy $\langle E^v_\alpha \rangle$ curves at different eigenenergies are similar except the one at the band center, so we will discuss only two energies as examples, one that is away from the band center and one very close to the band center.

### A. Eigenenergies away from the band center

We first study the von Neumann entropy $\langle E^v_\alpha \rangle$ and related quantities for eigenstates with eigenenergies $\varepsilon_\alpha \in [-0.84 - 0.02, -0.84 + 0.02]$. The literatures $11,14,15,16,17$ agree on the QP threshold $p_q \geq p_c \simeq 0.593$ if $p_q$ exits, where $p_c$ is the classical percolation threshold$13$. Therefore, we study the QP model at the site occupation probability $p$ beginning from 0.4, which is far smaller than the lower bound of $p_q$.

In Fig.3(a), we show the dependence of $\langle E^v_\alpha \rangle$ on the site occupation probability $p$ at system sizes $L = 20, 30, ..., 60$, respectively. It shows that $\langle E^v_\alpha \rangle$ monotonically increases as $p$ becomes larger. For a certain system size, when $p$ is small, e.g., $p = 0.4$, the eigenstates are...
localized and $\langle E_\alpha^0 \rangle$ is small. When $p = 1.0$, the model shown in Eq. (2) is a two-dimensional periodic potential system. Due to the Bloch theorem the eigenstate of a tight-binding electron on a local regular lattice is always in the extended state. At the situation, $\langle E_\alpha^0 \rangle$ is largest. All these reflect the trivial delocalization effect of $p$, which is similar as that studied in quantum small-world network models. All data shown in Fig. 3(a) are well fitted with nonlinear Boltzmann functions for various system sizes. According to the fitted lines, we plot the derivative $d(E_\alpha^0)/dp$ varying with $p$ in Fig. 3(b). It shows there is a peak in the derivative at a certain $p$, which is denoted by $p_{\text{max}}$. The maximal derivative and $p_{\text{max}}$ increase with the system sizes $L$, respectively. It is believed that the von Neumann entropy may be non-analytic at a quantum phase transitions and can reflect various quantum critical points. Therefore, that the derivative is maximal at a certain position $p_{\text{max}}$, can be as a signature of LDTs of electron states.

To study the LDTs at the QE threshold $p_q$, one needs to investigate the behavior of systems in the thermodynamic limit. However, in most cases this is not possible in numerical methods, and therefore, similarly as in Ref.[27], an extrapolation method is chosen. Fig. 3(c) shows the scaling behavior of the $p_{\text{max}}$. The $p_q$ in the thermodynamic limit can be obtained by $1/L \rightarrow 0$ and Fig. 3(c) shows $p_q \approx 0.676$ at the situation. We denote the derivative of von Neumann entropy at $p_{\text{max}}$ as $d(E_\alpha^0)/dp|_{p_{\text{max}}}$. Following the Refs. [33] and [34], the finite size scaling is performed for the function $1 - \exp(d(E_\alpha^0)/dp - d(E_\alpha^0)/dp|_{p_{\text{max}}})$ with respect to $L^{1/\nu}(p - p_{\text{max}})$. The result is presented in Fig. 3(d). It shows numerical results obtained from various system sizes approximately collapse on a single curve with the critical exponent $\nu \approx 2.52$.

**B. Eigenenergies near the band center**

In the following, we discuss the von Neumann entropy $\langle E_\alpha^\nu \rangle$ for eigenstates with eigenenergies $\epsilon_\alpha \in [0 - 0.02, 0 + 0.02]$. The von Neumann entropy $\langle E_\alpha^\nu \rangle$ and the corresponding derivative $d(E_\alpha^\nu)/dp$ varying with the site occupation probability $p$ are shown in Figs. 4(a) and (b), respectively. Fig. 4(a) shows that $\langle E_\alpha^\nu \rangle$ first increases with $p$ until to a plateau at $p \in [0.6, 0.85]$, then continues to increase, which is quitly different from that shown in Fig. 3(a) for eigenenergies away from the band center. Fig. 4(b) shows that the derivative $d(E_\alpha^\nu)/dp$ drastically decreases near $p \approx 0.6$ and drastically increases near $p \approx 0.85$.

With a real-space renormalization-group method, Odagaki and Chang observed three regimes of the electronic properties in QP models, which divided by the classical percolation threshold $p_c$, and the quantum percolation threshold $p_q(p_q > p_c)$. When $p < p_c$, electrons cannot tunnel between different isolated clusters and electrons are considered to be localized in the classical sense even in the quantum case. When $p_c < p < p_q$, due to

![FIG. 3: Some quantities for eigenstates with eigenenergies $\epsilon_\alpha \in [-0.84 - 0.02, -0.84 + 0.02]$. (a) The von Neumann entropy $\langle E_\alpha^\nu \rangle$ varying with the site occupation probability $p$ and the lines are Boltzmann fitting. (b) The derivative $d(E_\alpha^\nu)/dp$ varying with $p$. (c) The line corresponds to the expected behavior of $p_{\text{max}}$ for $1/L \rightarrow 0$ according to a second-order polynomial fitting. (d) The finite-size scaling analysis. The system sizes $L = 20, 30, ... , 60$ and the arrow direction in (a) and (b) denotes the increasing of $L$.](image)
to quantum interference effects, electrons cannot spread infinitely even there is an infinitely extended channel. The regime is called quantum localization regimes. When \( p > p_q \), electrons can spread infinitely and electron states are extended. They found \( p_c = 0.618 \) and \( p_q = 0.867 \). It is interesting that the von Neumann entropy \( \langle E_\alpha^v \rangle \) drastically changes near the two \( p \) values.

### C. Phase diagram

We have studied and extensively analyzed the von Neumann entropy for all the other eigenstates. As the system in Eq. (2) is bipartite, \( \varepsilon_\alpha \) and \( -\varepsilon_\alpha \) are both eigenvalues of \( \hat{H}_{A,B} \). Therefore we will restrict our investigation to one (left) half side of the band, i.e., \(-4 < \varepsilon_\alpha < 0\). Fig. 4(a) presents the phase diagram of LDTs in the \( \varepsilon_\alpha - p \) plane. The values of \( p \) at the LDTs are the QP threshold \( p_q \), which is obtained by the extrapolation method similarly as that shown in Fig. 3(c). The trend for \( p_q \) varying with \( \varepsilon_\alpha \) is similar as that for 2D quantum bond-percolation models on square lattices and 3D quantum site-percolation models on simple cubic lattice. In detail, we observe the nonmonotonic dependence of the values of \( p_q \) on eigenenergies \( \varepsilon_\alpha \). Notice that in the region \(-2t < \varepsilon_\alpha < -0.5t\) the QP threshold \( p_q \) are nearly constant and a weak maximum at \( \varepsilon_\alpha \simeq -t \), which are very similar as that found in Ref. [3]. That a weak maximum for \( p_q \) at \( \varepsilon_\alpha \simeq -t \) has also been found and discussed in Ref. [8], which may be due to the existence of von Howe singularity at the energy \( E_\alpha \). We find all the QP threshold \( p_q \) are greater than the classical percolation threshold \( p_c \simeq 0.593 \) and the lowest value \( p_q \simeq 0.665 \). As shown in Fig. 4(a), the phase diagram is very consistent with the mobility edge trajectory shown in Ref. [13] for the same model obtained by the Thouless-Edwards-Llicciardello method.

Fig. 4(b) presents all the critical exponents \( \nu \) versus eigenenergies \( \varepsilon_\alpha \) according to the finite scaling analysis similarly as that shown in Fig. 4(d). We find the values of \( \nu \) depend on eigenenergies \( \varepsilon_\alpha \). In detail, in the region \(-2t < \varepsilon_\alpha < -0.5t \) where \( p_q \) are almost constant(see Fig. 4(a)), most of the values of \( \nu \) are distributed in a relatively narrow interval \([2, 3]\). From the band edge to \( \varepsilon_\alpha \simeq -2t \), \( \nu \) increase with \( \varepsilon_\alpha \), while from \( \varepsilon_\alpha \simeq -0.5t \) to the band center, \( \nu \) decrease with \( \varepsilon_\alpha \). All \( \nu \) are larger than \( 2/D(D = 2) \), which satisfies the assumption that \( \nu \) must satisfy the bound \( \nu > 2/D \) for random systems. Though \( \nu \) has been extensively studied in 3D QP models, to our best knowledge, there are few works to study \( \nu \) in 2D QP models except in Ref. [14], where the critical exponent for correlation lengths \( \nu \simeq 3.3 \). The varying of the critical exponent \( \nu \) with the QP threshold \( p_q \) is plotted in Fig. 4(c). It shows near the band edge and near the band center the relation between \( \nu \) and \( p_q \) is linear, respectively, but the linear relations are different. This may be caused by the different symmetry and/or degeneration at the two energy regions.

### IV. CONCLUSIONS AND DISCUSSIONS

In this paper, we have detailed studied the von Neumann entropy \( \langle E_\alpha^v \rangle \) varying with eigenenergies \( \varepsilon_\alpha \) and accessible site concentrations \( p \) by quantum particles in two-dimensional quantum site-percolation models on square lattices.

For Eigenenergies away from the band center, we determine the QP threshold \( p_q \) by the derivative of von Neumann entropy is maximal at the point. Based on this, we give the phase diagram of LDTs in the \( \varepsilon_\alpha - p \) plane, which is very consistent with the mobility edge trajectory shown in Ref. [13]. From the phase diagram, we observe the nonmonotonic eigenenergies dependence of \( p_q \) and the lowest value \( p_q \approx 0.665 \). At the same time, the finite-size scaling analysis is performed at all LDTs points. To the best of our knowledge, it is the first time to obtain all the critical exponents \( \nu \) at the whole energy space for 2D QP models. We find the critical exponents \( \nu \) depend on eigenenergies \( \varepsilon_\alpha \).

For eigenenergies near the band center, the variations of the von Neumann entropy \( \langle E_\alpha^v \rangle \) with respect to \( p \)
for are quite different from that for eigenenergies away from the band center. It can reflect the classical percolation threshold \( p_c \) and the QP threshold \( p_q \) for eigenenergies at the band center.

All our numerical results show that there is \( p_q < 1 \) in 2D QP models and \( p_q \) depends on eigenenergies. The debates on the values of \( p_q \) may be partially due to different energies treated in literatures.

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