von Neumann entropy and localization-delocalization transition of electron states in quantum small-world networks

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The von Neumann entropy for an electron in periodic, disorder, and quasiperiodic quantum small-world networks (QSWN's) is studied numerically. For the disorder QSWN's, the derivative of the spectrum-averaged von Neumann entropy is maximal at a certain density of shortcut links p^*, which can be as a signature of the localization-delocalization transition of electron states. The transition point p^* is agreement with that obtained by the level statistics method. For the quasiperiodic QSWN's, it is found that there are two regions of the potential parameter. The behaviors of electron states in different regions are similar to that of periodic and disorder QSWN's, respectively.

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I. INTRODUCTION

Recently the small-world networks (SWN's) [1] have attracted much attention since they can mimic social and biological networks, Internet connections, airline flights, and other complex networks. Well-established classical models have been numerically and analytically investigated, which focused on the crossover behavior [2], the scaling properties [3,4], the percolation of the dynamic processes [4] in the model, etc. Very recently Zhu and Xiong have generalized the SWN's to a quantum version by regarding the bonds as quantum hopping links for the motion of an electron and investigated the localization-delocalization transition of electron states [5]. Until now the transition point has been found only by using the level statistics method combined with the finite-size scaling method [5–7]. However, the finite-size scaling method is not suitable for SWN's with high connections since the number of connections grows very rapidly with the SWN size [7]. The level statistics method is successful in the location of the metal-insulator transition in disorder systems [8,9], but it is not suitable in quasiperiodic systems because the level spacing distribution [10] cannot always be written as the crossover of the Poisson distribution and Wigner-Dyson distribution.

On the other hand, the connection between the entanglement (such as von Neumann entropy) and localization properties of eigenstates has been revealed recently. By measuring the von Neumann entropy, the local entanglement was studied at the ground state in the Hubbard model for the dimer case [11] and in the extended Hubbard model for different band fillings [12]. It is found that the von Neumann entropy is suitable to describe quantum phase transitions [12] and analyze the interplay between itinerant and localized features [11].

In this paper, we study the von Neumann entropy for an electron moving in periodic, random, and quasiperiodic quantum small-world networks (QSWN's), respectively. In periodic QSWN's, there are no localization-delocalization transitions because all eigenstates are extended. In random QSWN's, we find that the spectrum-averaged von Neumann entropy is a suitable quantity to analyze the localization-delocalization transition of electron states. Finally, we propose quasiperiodic QSWN's based on the one-dimensional Harper model. With the help of von Neumann entropy, we find that there are two regions of the potential parameter in the model. The behaviors of electron states in different regions are similar to that of periodic and disorder QSWN's, respectively.

The paper is organized as follows. In the next section we describe the QSWN model and the measure of entanglement. In Sec. III we present numerical results for different QSWN's. Finally, in Sec. IV, the conclusions are given.

II. MODEL AND VON NEUMANN ENTROPY

We consider a circular graph with N vertices. Each vertex is linked with (direct connections) its two nearest neighbors. To this graph, pN shortcut links (connecting $2pN$ vertices) are additionally added between random pairs of vertices without direct connections (Fig. 1) [4]. Here p is the density of shortcut links.

The tight-binding Hamiltonian of an electron in QSWN's can be written as

$$H = H_0 + H_1, \tag{1}$$

where

$$H_0 = t\sum_{n=1}^{N} (c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n) + \sum_{n=1}^{N} \varepsilon_n c_n^\dagger c_n \tag{2}$$

and

$$H_1 = t_1 \sum_{k=1}^{pN} \sum_{n=1}^{N} \sum_{m=1}^{N} (c_n^\dagger c_m + c_m^\dagger c_n)\delta_{n,n_k}\delta_{m,m_k}. \tag{3}$$

Here t is a nearest-neighbor hopping integral, $c_n^\dagger$ (c_n) the creation (annihilation) operator of the nth site, and ε_n the on-site potential. It is clear that the H_0 defines a one-

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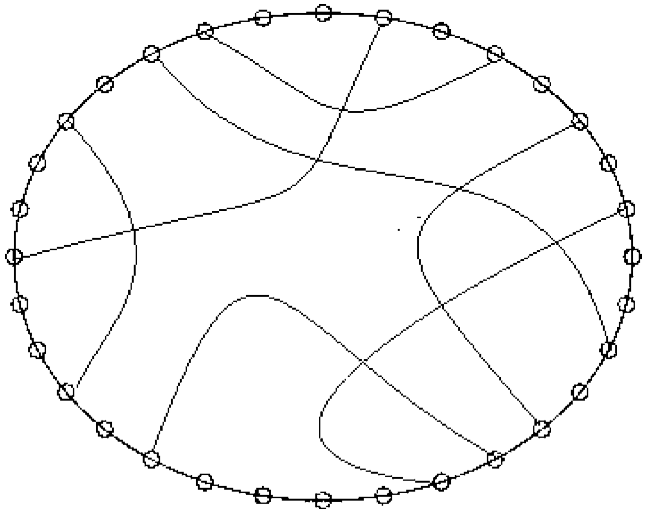

FIG. 1. An example of a small-world graph with vertices $N=32$ and shortcut links $pN=7$.

dimensional tight-binding model. t_1 is the hopping integral for shortcut links; $\{n_k,m_k\}$ (here we impose the restriction that $n_k<m_k$) are the pairs of vertices connected by a shortcut link, and the number of all pairs is pN. Theoretically, $(pN)_{max}=N(N-3)/2$. Here we only study small values of p.

Let $|n\rangle \equiv c_n^\dagger|0\rangle$; the general eigenstate of an electron is

$$|\alpha\rangle = \sum_{n=1}^{N} \psi_n^\alpha |n\rangle = \sum_{n=1}^{N} \psi_n^\alpha c_n^\dagger |0\rangle, \tag{4}$$

where ψ_n^α is the amplitude of wave function α at the nth site.

The general definition of entanglement is based on the von Neumann entropy [13]. For an electron in the system, there are two possible local states at each site, $|1\rangle_n$ and $|0\rangle_n$, corresponding to the state with (without) an electron at the nth site, respectively. The local density matrix ρ_n is defined [11,12] by

$$\rho_n = z_n|1\rangle_{nn}\langle 1| + (1-z_n)|0\rangle_{nn}\langle 0|, \tag{5}$$

where $z_n=\langle\alpha|c_n^\dagger c_n|\alpha\rangle=|\psi_n^\alpha|^2$ is the local occupation number at the nth site. The corresponding von Neumann entropy is

$$E_{vn}^\alpha = -z_n \log_2 z_n - (1-z_n)\log_2(1-z_n), \tag{6}$$

which measures the entanglement of states on the nth site with that on the remaining $N-1$ sites. It is called the local entanglement for it exhibits correlations between a site and all the other sites of the system [11,12]. Generally E_{vn}^α is a function of n. We define the von Neumann entropy of system at α eigenstate as

$$E_v^\alpha = \frac{1}{N}\sum_{n=1}^{N} E_{vn}^\alpha. \tag{7}$$

The definition (7) shows that for an extended state $\psi_n^\alpha=\frac{1}{\sqrt{N}}$ for all n, $E_v^\alpha=-\frac{1}{N}\log_2\frac{1}{N}-(1-\frac{1}{N})\log_2(1-\frac{1}{N})\approx\frac{1}{N}\log_2 N$ at $N\to\infty$, and for a localized state $\psi_n^\alpha=\delta_{nn^0}$ (n^0 is a given site), $E_v^\alpha=0$. In this paper all the values of E_v^α and E_{vn}^α are scaled by $\frac{1}{N}\log_2 N$. From the two examples, we know that the scaled E_v^α is near 1 when eigenstates are extended and near zero when eigenstates are localized. Henceforth, we omit "scaled" for simplicity.

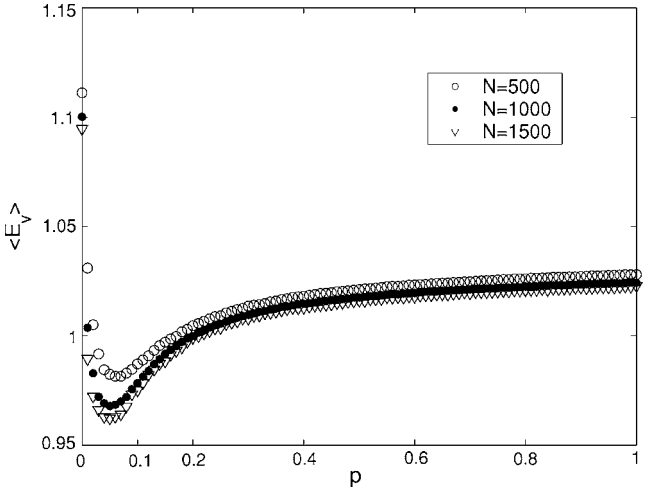

FIG. 2. The spectrum-averaged von Neumann entropy $\langle E_v\rangle$ varying with p at different sizes N for periodic QSWN's.

As a further gross measure we also average over all the eigenstates—i.e., the spectrum-averaged von Neumann entropy

$$\langle E_v\rangle = \frac{1}{M}\sum_{\alpha} E_v^\alpha, \tag{8}$$

where M is the number of all eigenstates.

III. NUMERICAL RESULTS

In our numerical calculations, the Hamiltonian is obtained according to the formulas (1)–(3) for finite systems. The shortcut terms are generated randomly based on formula (3). We directly diagonalize the Hamiltonian and obtain N eigenvalues E_α and corresponding eigenvectors $|\alpha\rangle$. From the formulas (5)–(8), we obtain the spectrum-averaged von Neumann entropy $\langle E_v\rangle$ for one realization of QSWN's. The results are averaged over many realizations of QSWN's.

A. Periodic QSWN's

For periodic QSWN's, the on-site potential ε_n is assumed to be uniform and set equal to zero. Without loss generality and for simplicity, we set $t=t_1=1$ in all our numerical calculations. Figure 2 shows the spectrum-averaged von Neumann entropy $\langle E_v\rangle$ changing with p at $N=500$, 1000, and 1500, respectively. Averages are done for 300, 200, and 100 random configurations (positions of shortcut links) at $N=500$, 1000, and 1500, respectively. The results are similar for more random configurations. From the figure, we can see that $\langle E_v\rangle$ is close to 1 for all p, which means that all states are extended and there is no localization-delocalization transition in the systems. For $p=0$—i.e. in the absence of shortcuts—the model is a one-dimensional periodic potential system. The energy eigenstates are always extended due to the Bloch theorem. The random shortcut terms can cause long-range

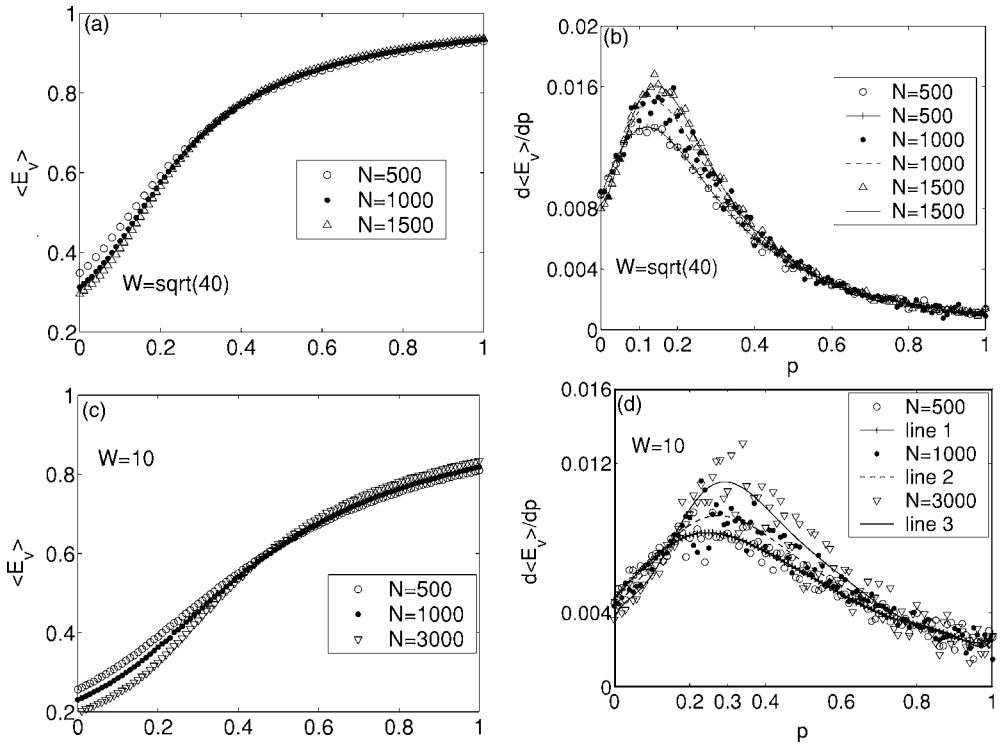

FIG. 3. The spectrum-averaged von Neumann entropy $\langle E_v \rangle$ (a),(c) and the derivative $d\langle E_v \rangle / dp$ (b),(d) varying with p at different sizes N for $W=\sqrt{40}$ (a),(b) and $W=10$ (c),(d), respectively. Lines in figures are polynomial fitted for corresponding data. The number of disorder realizations (positions of shortcut links and on-site disorder potential) is 300, 200, 100, and 20 for $N=500$, 1000, 1500, and 3000, respectively.

hopping and off-diagonal disorder effects. Long-range hopping tends to delocalize the states; therefore, the extensive properties of the eigenstates are not changed by the presence of random shortcut terms. We also find there is small decreases of $\langle E_v \rangle$ for *very small* p ($p<0.05$), which is due to localization effects of the off-diagonal disorder caused by random shortcut terms in the Hamiltonian.

B. Disordered QSWN's

For disordered QSWN's, the on-site potentials ε_n are random variables homogeneously distributed with $[-W/2; W/2]$. Here W characterizes the degree of on-site disorder as in the Anderson model [14]. By using the level statistics method, it has been found that a transition from Possion statistics (localized phase) to Wigner-Dyson statistics (delocalized phase) takes place at $p_c \approx 1/400(W/t)^2$ for weak disorder; i.e., W/t is small [6].

In Fig. 3 we show the spectrum-averaged von Neumann entropy $\langle E_v \rangle$ and the derivative $d\langle E_v \rangle / dp$ varying with p for $W=\sqrt{40}$ and $W=10$ at different N, respectively. From 3 (A) and (C), it is clear that $\langle E_v \rangle$ monotonically increases as p becomes larger. When $p=0$, the model is a one-dimensional Anderson model [14]. For the model all states are localized, so $\langle E_v \rangle$ are small ($\langle E_v \rangle \approx 0.3$ and 0.2 at $W=\sqrt{40}$ and 10, respectively). When p is large, delocalized states will be present due to the long-range hopping and $\langle E_v \rangle$ becomes large. From Figs. 3(b) and 3(d), it is found that the derivative $d\langle E_v \rangle / dp$ is maximal at $p^* \approx 0.1-0.15$ and 0.25–0.3 at $W=\sqrt{40}$ and $W=10$, respectively. The p^* is agreement with the localization-delocalization transition point p_c obtained by the level statistics method ($p_c \approx 0.1$ at $W=\sqrt{40}$ and $p_c \approx 0.25$ at $W=10$) [6]. It is clear that the transition from the localized phase to the delocalized phase can also be reflected from $d\langle E_v \rangle / dp$. Therefore the von Neumann entropy is a suitable quantity to analyze localized properties of electron states for QSWN's.

C. Quasiperiodic QSWN's

After the experimental discovery of the quasicrystals [15] and one-dimensional quasiperiodic superlattices [16], many experimental and theoretical works have been carried out on the physical properties of quasiperiodic systems [17–23]. Although these systems lack translational invariance, they are perfectly ordered. In this sense, such systems can be regarded as intermediate between periodic and random systems. One of the most popular quasiperiodic systems is the Harper model. In the following, we propose a quasiperiodic QSWN based on the Harper model and study the properties of the eigenstates of an electron in this system.

For the Harper quasiperiodic QSWN's, we choose $\varepsilon_n = \lambda \cos(2\pi\sigma n)$ and σ is irrational. The potential is incommensurate with the underlying vertices. At $p=0$ the model is in fact the one-dimensional well-studied Harper model [17]. Intensive analytical and numerical studies [17–23] for the Harper model show that for $\lambda < 2$ the spectrum becomes continues and all eigenstates are extended. For $\lambda > 2$ the spec-

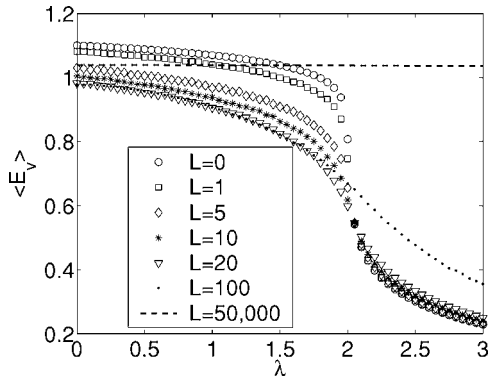

FIG. 4. The spectrum-averaged von Neumann entropy $\langle E_v \rangle$ varying with λ at different shortcut link numbers L. Here $N=987$ and the number of random configurations (positions of shortcut links) is 200.

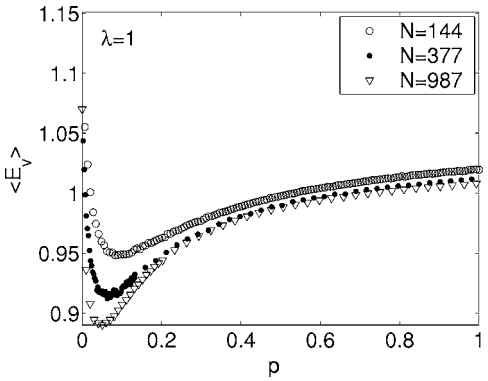

FIG. 5. The spectrum-averaged von Neumann entropy $\langle E_v \rangle$ as a function of p at $\lambda=1$ for different system sizes. The number of random configurations (positions of shortcut links) is 500, 300, and 200 for $N=144$, 377, and 987, respectively.

trum is pure point and all eigenstates are exponentially localized. For $\lambda=2$ the situation gives the metal-insulator transition at which the eigenstates are neither extended nor localized but critical with a singular-continuous multifractal spectrum.

As a typical case, we take $\sigma=(\sqrt{5}-1)/2$. In fact, as is customary in the context of quasiperiodic systems, the value of σ may be approximated by the ratio of successive Fibonacci numbers: $F_n=F_{n-2}+F_{n-1}$. In this way, choosing $\sigma=F_{n-1}/F_n \approx (\sqrt{5}-1)/2$ and system size $N=F_n$, we can obtain the periodic approximant for the quasiperiodic potential [23].

In Fig. 4, we plot the spectrum-averaged von Neumann entropy $\langle E_v \rangle$ varying with λ for different shortcut link numbers L (here $L=pN$). For $L=0$, $\langle E_v \rangle$ is large at $\lambda<2$, while small at $\lambda>2$. There is a sharp decrease in $\langle E_v \rangle$ for $\lambda=2$; i.e., the absolute value of $d\langle E_v \rangle/dp$ is maximal at $\lambda=2$, so the metal-insulator transition can be reflected from $\langle E_v \rangle$. When L is small ($L \leqslant 20$), those varying properties of $\langle E_v \rangle$ are similar to that for $L=0$, which means that at small L, the quasiperiodic on-site potentials rather than shortcut links play an important role. When L is large ($L=100$), the decrease in $\langle E_v \rangle$ at $\lambda=2$ is not so sharp as that for $L \leqslant 20$. When L is large enough (for example, $L=50\,000$), $\langle E_v \rangle$ is almost same for all λ. In this situation the SWN's form almost completely a random graph and the on-site potential is not important.

For $\lambda<2$, the varying properties of $\langle E_v \rangle$ with p are similar to that of periodic QSWN's. In Fig. 5, $\lambda=1$ is given as an example. It shows that on the whole, for all p, $\langle E_v \rangle$ is near 1, which means all states are extended.

For $\lambda>2$, the varying properties of $\langle E_v \rangle$ and the derivative $d\langle E_v \rangle/dp$ with p are similar to those for disorder QSWN's. In Fig. 6, $\lambda=3$ and 5 are examples. The spectrum-averaged von Neumann entropy $\langle E_v \rangle$ and the derivative $d\langle E_v \rangle/dp$ with different p are shown in Figs. 6(a) and 6(b), respectively. It shows that $\langle E_v \rangle$ monotonically increases as p increases. The derivative $d\langle E_v \rangle/dp$ is maximal at $p^* \approx 0.12$ and 0.4 at $\lambda=3$ and 5, respectively, so the localization-delocalization transition happens at p^*. This also can be certified by the level statistics method.

To understand the effect of shortcut links clearly, in Figs. 7(a), 7(b), and 7(c) we plot the average von Neumann entropy $\langle E_v^\alpha \rangle$ of the individual eigenstates at $\lambda=1$, 2, and 3 for $L=0$, 20, and 100, respectively. When $\lambda=1$, at $L=0$ all $\langle E_v^\alpha \rangle$ are large (near 1), which corresponds to the fact that all eigenstates are extended. At $L=20$, the subband created by the shortcut links lies below the band bottom, above the band top, and at the band gap of that for $L=0$. In those newly created subbands, $\langle E_v^\alpha \rangle$ are obviously small compared to that for $L=0$, which means shortcut links can produce localized

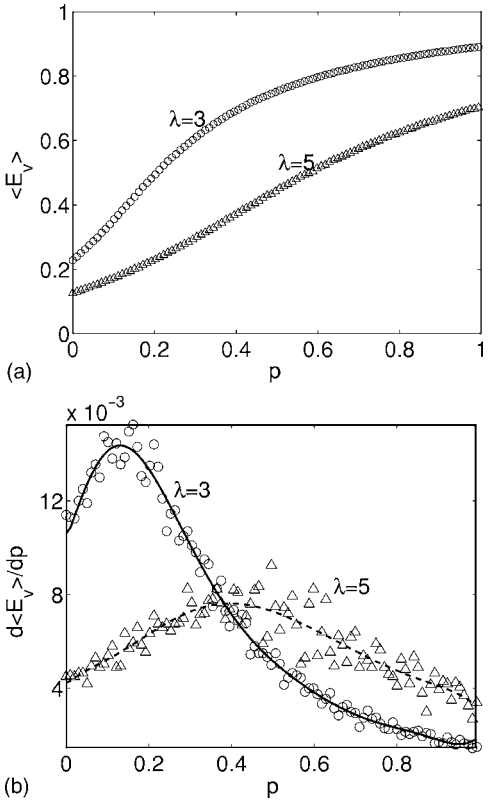

FIG. 6. The spectrum-averaged von Neumann entropy $\langle E_v \rangle$ and $d\langle E_v \rangle/dp$ varying with the density of shortcut links p for (a) and (b), respectively. Lines in the figure are polynomial fitted for the corresponding data. Here $N=987$ and the number of random configurations (positions of shortcut links) is 200.

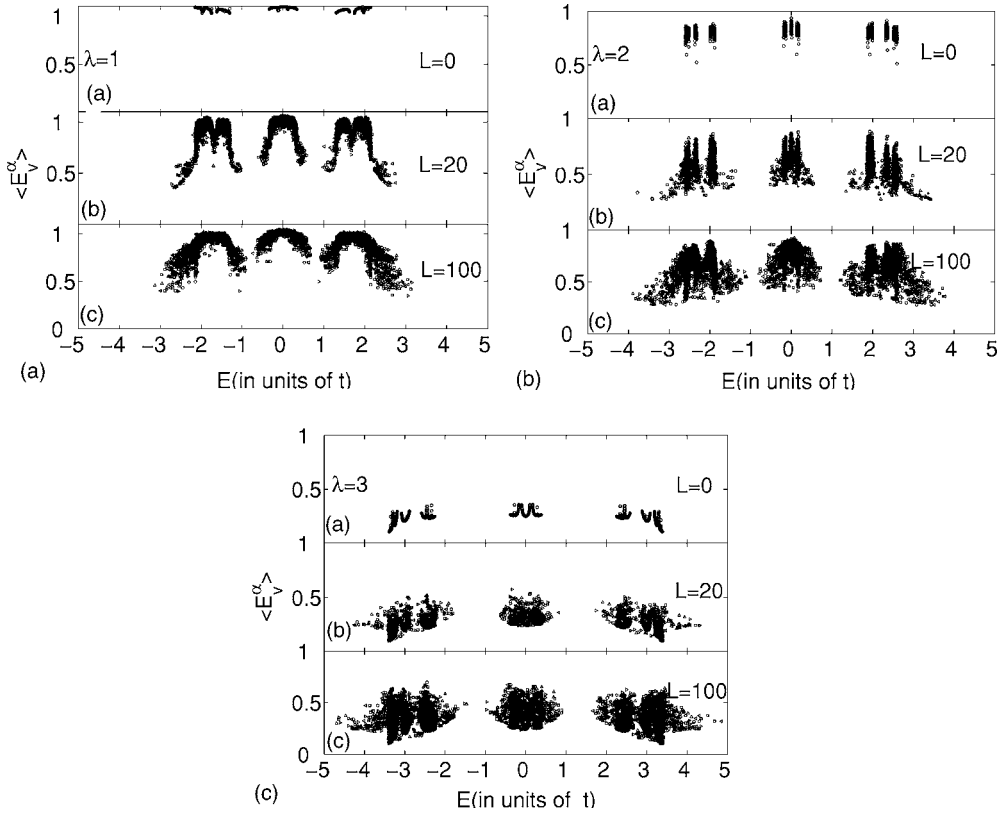

FIG. 7. Average von Neumann entropy $\langle E_v^\alpha \rangle$ of the individual eigenstate as functions of eigenenergies at $L=0$, 20, and 100 for (a) $\lambda=1$, (b) $\lambda=2$, and (c) $\lambda=3$, respectively. For $L>0$, the $\langle E_v^\alpha \rangle$ values for six random configurations (positions of shortcut links) of quasiperiodic QSWN's are plotted together. Here $N=987$.

states at the case. As L increases to 100 and the long hopping becomes more and more important, on the whole $\langle E_v^\alpha \rangle$ in the newly created subbands are larger than that for $L=20$. When $\lambda=3$, at $L=0$ all $\langle E_v^\alpha \rangle$ are small comparing to that for $\lambda=1$ at $L=0$, which corresponds to the fact that all eigenstates are localized. At $L>0$, $\langle E_v^\alpha \rangle$ for most eigenstates are large compared with that at $L=0$. In this situation the long hopping due to shortcut links is important and makes many states more extended than that at $L=0$. When $\lambda=2$, at $L=0$ the eigenstates are critical with a singular-continuous multifractal spectrum. In this situation some eigenstates have large $\langle E_v^\alpha \rangle$ and some have small $\langle E_v^\alpha \rangle$. At $L=20$, $\langle E_v^\alpha \rangle$ become larger at some eigenstates and smaller at some eigenstates due to the shortcut links. The spectrum-averaged von Neumann entropy $\langle E_v \rangle$ changes little. At $L=100$, the long hopping becomes important and leads to many eigenstates having large $\langle E_v^\alpha \rangle$ compared to that for $L=20$.

IV. CONCLUSIONS

In detail, we study von Neumann entropy in periodic and disorder QSWN's and find it is a suitable quantity to reflect the localization-delocalization transition of electron states. Then we propose a quasiperiodic QSWN based on the one-dimensional Harper model and investigate it intensively by the measure of von Neumann entropy. In the model, the quasiperiodic on-site potential, the long-range hopping, and off-diagonal disorder due to random shortcut links determine the localization properties of electron states. Those lead to the conculsion that the influence of shortcut links on the von Neumann entropy is different at two λ regions ($\lambda<2$ and $\lambda>2$). We found that when $\lambda<2$, on the whole, for all p, $\langle E_v \rangle$ is near 1, which means all states are extended. When $\lambda>2$, it monotonously increases as p is increased. Those can be understood from varying the average von Neumann entropy $\langle E_v^\alpha \rangle$ of the individual eigenstates with λ and the number of shortcut links. Especially, at $\lambda>2$ we find that there exists a localization-delocalization transition of electron states reflected from the von Neumann entropy. In a word, the varying of $\langle E_v \rangle$ with p is similar to that for periodic QSWN's at $\lambda<2$ and similar to that for disorder QSWN's at $\lambda>2$.

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