Fractal analysis of wave functions at the localization-delocalization transition in a disordered quantum small-world-network model

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Localization-delocalization transition in disordered quantum small-world network model is confirmed by using the numerical multifractal analysis of the wave functions at the critical point. A linear relation between the numerator and the denominator of the parametric representation for the singularity spectrum of the wave functions near the transition point is obtained, serving as a criterion of the critical behavior. The singularity spectrum $f(\alpha)$ at the critical point is size independent. The variation of the fractal intensity α_q at $q=0$ and $q=1$ in changing the rewiring probability p reveals the phase transition as shown in the level statistics on the same model.

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Localization-delocalization transition (LDT) in low-dimensional systems has attracted considerable attention for a long time due to the importance in theoretical and experimental investigations of the condensed-matter physics. From the scaling theory the LDT can occur only in systems of dimensionality greater than 2.[1] Thus, it is interesting to construct systems with varying dimensionality and to investigate the LDT in them. Recently, the small-world-network (SWN) model has been proposed and studied in its classical aspect.[2] Since the effective dimensionality of SWN depends on the probability of the bond rewiring p, it can serve as a suitable model to study the LDT in systems with varying dimensionality. For this purpose we have generalized the one-dimensional (1D) SWN to its quantum version by regarding the bonds as quantum hopping links for the motion of electrons and investigated the LDT of electronic states by adding the diagonal disorder of the site energies.[3] Our numerical calculations on the level statistics demonstrate that there does exist LDT in increasing p due to the competition between the enhancement of the effective dimensionality and the disorder of topology and site energies. Critical point p_c is determined by the finite-size scaling for the level statistics, and a universal distribution function is found at the critical point.[3]

On the other hand, it is commonly believed that the wave functions near the critical point of LDT exhibit multifractality. Aoki has pointed out that the wave function at the Anderson transition corresponding to the fixed point in a real-space renormalization-group study should be scale invariant and exhibit self-similarity.[4] Schreiber and Grussbach found that at the critical point of the 3D Anderson model, strong spatial fluctuations of the amplitudes of the wave function display the multifractal character on all length scales.[5] They showed that the singularity spectrum of the critical wave function does not depend on the system size and rather takes a universal form. Furthermore, they assumed that the singularity spectrum is universal for the LDT, regardless of the specific values of parameters of models, and from this they established a straightforward method to distinguish the localized and extended states.

In this paper we investigate the multifractality properties of the wave function at the LDT in disordered quantum small world (DQSW) model. We obtain a universal singularity spectrum $f(\alpha)$ that features the critical wave functions. We find that the localization degree of states in the DQSW model can be characterized by several discrete multifractal intensities. The form of singularity spectra, independent of the size and other parameters, further confirms the existence of LDT in DQSW systems.

We consider a 1D ring with N sites and even coordination number Z. In the initial structure every site links with its $Z/2$ neighboring sites with direct bonds on every side. Then one performs the rewiring process that every bond starting from a site labeled as i has a probability p to be broken and rewired to another randomly chosen site other than the Z neighboring sites of i. After this procedure applied on all the sites a so-called small-world-network[2] is created that is topologically random but may have an effective dimensionality higher than 1 due to the cutoff paths via the rewired bonds. In the quantum version every site has been assigned an electron orbital and every bond represents the hopping integral between two orbitals on its ends. We also introduce the diagonal disorder with a uniform distribution in the range of $[-w/2,w/2]$ for the orbital levels on the sites. Thus, the tight-binding Hamiltonian of the DQSW model reads

$$H=\sum_{i=1}^{N}\epsilon_i|i\rangle\langle i|+\sum_{i=1}^{N}\sum_{l=1}^{Z/2}[t_1(1-\rho_{i,l})(|i\rangle\langle i+l|+|i+l\rangle\langle i|) + t_2\rho_{i,l}(|i\rangle\langle i_R|+|i_R\rangle\langle i|)], \quad (1)$$

where i_R represents a randomly chosen site other than the Z neighboring sites of site i and subject to the restriction that there are no repeating terms in the summation, $\rho_{i,l}$ is a random variable obeying the distribution function

$$P(\rho_{i,l})=\begin{cases} p, & \text{for } \rho_{i,l}=1, \\ 1-p, & \text{for } \rho_{i,l}=0, \end{cases}$$

the orbital level ϵ_i is randomly distributed between $-w/2$ and $w/2$ with a constant probability, and t_1 and t_2 are hopping integrals for the regular bonds and the rewired bonds, respectively.

The Hamiltonian can be numerically diagonalized to yield the wave functions for various parameters. We adopt the spatial distribution of amplitudes $|\psi_j(i)|^2$ of a wave function with eigenenergy E_j as the entity of the multifractal analysis to investigate its localization properties. In the calculation of the singularity spectrum we use the standard box-counting method.[6] In this method the entire circumference of the DQSW ring is divided into N_L ($N_L \leqslant N$) boxes of length L. The probability to find an electron in the kth box is given by

$$\mu_{k,j}(L) = \sum_{i \in k} |\psi_j(i)|^2, \quad \text{for} \quad k = 1,2,3,\ldots,N_L. \tag{2}$$

In the statistical sense $\mu_{k,j}(L)$ depends on the size of boxes with a power-law relation. The singularity strength α_k in the kth box is defined as the exponent of the power law

$$\mu_k(L) \sim L^{\alpha_k}. \tag{3}$$

Here we omit the index of the wave function for the simplicity. Thus, the boxes can be grouped into several subsets according to the values of α_k. The subset α contains the boxes with α_k within a window of α. The number density $N(\alpha)$ of subset α is a fractal itself with the Hausdorff dimension $f(\alpha)$

$$N(\alpha, L) \sim L^{-f(\alpha)}. \tag{4}$$

The singularity spectrum $f(\alpha)$ completely characterizes the multifractality of the whole measure of the probability distribution of the wave function. In order to avoid suffering from the possible numerical inaccuracies in the Legendre transformation, many authors employ a parametric representation[6] of $f(\alpha)$ in terms of q. Namely, one can use the properly normalized qth moment of the spatial distribution of the wave function to constitute a measure

$$\mu_k(q,L) = \mu_k^q(L) / \sum_{k'} \mu_{k'}^q(L). \tag{5}$$

Then $\alpha(q)$ and $f(q)$ are presented, respectively, in the following form:

$$\alpha(q) = \lim_{\delta \to 0} \sum_k \mu_k(q,L) \ln \mu_k(1,L) / \ln \delta, \tag{6}$$

$$f(q) = \lim_{\delta \to 0} \sum_k \mu_k(q,L) \ln \mu_k(q,L) / \ln \delta, \tag{7}$$

where $\delta = L/N$ denotes the ratio of the box size and the system size. However, as pointed out by several authors, Eq. (7) is valid only in the existence of a linear relation between the numerator and the denominator for different values of δ. We can define $v = \Sigma_k \mu_k(q,L) \ln \mu_k(q,L)$ and $x = \ln \delta$. Thus, in the procedure of $\delta \to 0$ in the relative sense (actually L cannot be shorter than the lattice spacing, 1) the linear relation v versus x in Eq. (7) reflects the scaling invariance of the measure of the fluctuations of the amplitudes of the wave function in all possible length scales. In fact, this behavior can serve as a criterion of the Anderson transition. Below we will use this criterion to study the localization properties of the wave functions.

In the numerical calculations we first use the value of p in the region far from the critical point p_c that was obtained in the scaling analysis of the level statistics.[3] No linear relation of $v(x)$ is found for the eigenfunctions near the center of the band in a system with size $N = 2400$. However, when we carry out the same calculations for p in the vicinity of p_c in a system with the same size, this linear relation of $v(x)$ indeed appears. Within the range of $p_c \pm 0.0005$, the wave functions near the band center all exhibit the anticipated linear characteristics of $v(x)$ [an example is shown in Fig. 1(a)]. In the calculations L scales from 2^0 to 2^n with $n \sim 5$ or 6 that are precise enough for system size $N \sim 10^3$. By changing the system size to $N = 1200$ and $N = 3600$ the good linear fitting persists, as shown in Figs. 1(b) and 1(c), respectively. Therefore, we can confirm that the multifractality of the wave functions near the critical point manifests itself for different system sizes.

The existence of the multifractality of the wave functions at the band center for specific values of p provides a new evidence for the LDT in the DQSW model. Moreover, the value of p_c from the multifractality analysis of the wave functions is consistent with that from the analysis of the level statistics. From these results a universal form of singularity spectra independent of the system size and the value of p_c is naturally expected.[7] This is confirmed in our calculations and the results for different size ($N = 1200$, 2400, 3600) and different coordinate number ($Z = 8$, 12) are shown in Fig. 2. Here p_c decreases by increasing Z as larger Z provides more opportunities for the shortcut paths. Curves of singularity spectra for various parameters are essentially coincident in the range of $0 < \alpha < 3.0$. A little diversity appears in the region of $\alpha > 3.0$, which corresponds to $q < 0$ with larger absolute value of q. Since q acts as a microscope of exploring the singularity measure in different regions of amplitudes of wave functions, the very small amplitudes of wave functions are amplified in the moment of a negative q with large absolute value, corresponding to the subsets with larger singularity strength α. In this region the calculated results are mostly sensitive to the numerical errors and the digit controlling, which lead to the unavoidable deviation from the exact behavior. We note that although the critical point p_c is different for different Z, the singularity spectrum near the critical point shows the same behavior. This implies that the critical singularity spectra are universal for the critical point of the DQSW model with different coordinate numbers. The shape of the curves is similar to that shown in Refs. 5 and 7. The only difference from the spectra of Refs. 5 and 7 is the scales of $f(\alpha)$ and α. In the present case the box counting is performed in 1D boxes while in Refs. 5 and 7 it is done in 3D boxes. Because α and $f(\alpha)$ are both fractal dimension of quantities obtained from the box counting, the scales of α and $f(\alpha)$ are approximately shrunk by 3 times in comparison with those in Refs. 5 and 7.

We also investigated the p dependence of the multifractal strength α_q for $q = 0$ and $q = 1$ in a system with a given size.

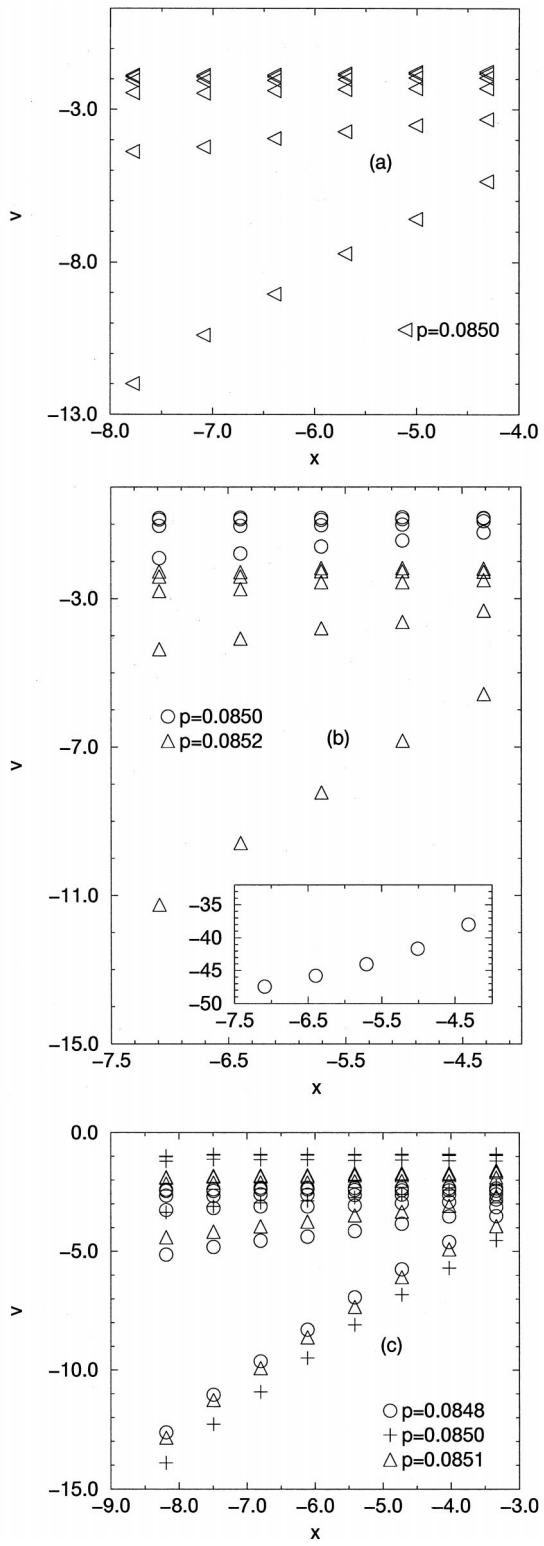

FIG. 1. (a) Dependence of $v \equiv \Sigma \mu(q,L) \ln \mu(1,L)$ on $x \equiv \ln \delta$ for wave functions near the band center of a DQSW system with p near the critical value. The other parameters are $Z=8$, $w=18.0$, $N=2400$, and $q=0,1,2,3,4,5$ (from bottom to top). (b) Relation of v to x with the same parameters as those in (a) but $N=1200$, and from bottom to top $q=0,1,2,3,4$ for $p=0.0852$ and $q=0,1,2,3$ for $p=0.0850$. Inset: $q=4$ for $p=0.0850$. (c) Relation of v to x with the same parameters as those in (a) but $N=3600$.

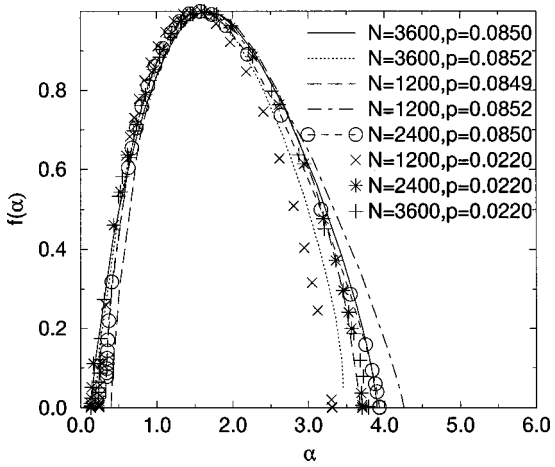

FIG. 2. Singularity spectrum $f(\alpha)$ as a function of α for wave functions of systems near the transition point p_c. For systems with coordinate number $Z=8$ the data are shown with both symbols and connecting lines, for system with $Z=12$ only the symbols are displayed.

The results are shown in Fig. 3. The two values exhibit opposite monotonous evolution in varying p. For the sake of clarity we plot two horizontal lines at values of $\alpha_1(p_c)$ and $\alpha_0(p_c)$ to divide the area into the localization districts outside the two lines and the delocalization one between them. When the rewiring probability p increases, both $\alpha_0(p)$ and $\alpha_1(p)$ cross the critical lines at the same value of p, corresponding to the transition from the localization to the delocalization. We observe that the difference $\Delta\alpha=\alpha_0(p)-\alpha_1(p)$ can reflect the localization degree even though the exact multifractality does not exist in systems far from the critical point. It is worth stressing that although all the calculations are carried out in a single configuration of the disorder and no ensemble average is taken, the smooth profile of the curves suggests the excellent self-averaging and that the multifractal analysis is an effective method in determining the localization-delocalization transition. Moreover, we

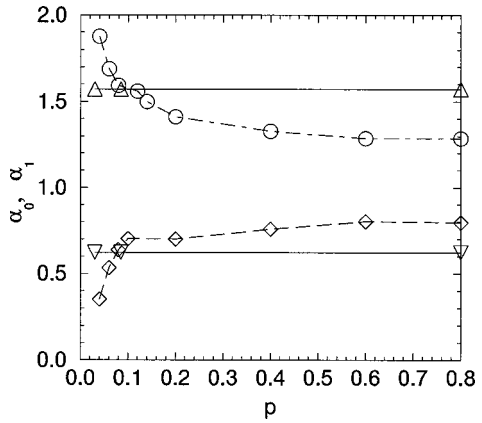

FIG. 3. Multifractal intensities α_0 ($\bigcirc$) and α_1 ($\diamond$) as functions of rewiring probability p. Two solid lines with upper and down triangle symbols correspond the reference values of α_0 and α_1 at the critical point p_c, respectively. The system size is $N=2400$ and the other parameters are the same as those in Fig. 1(a).

believe that a careful search for the linearity of function $v(x)$ is a key procedure for the reliability of the method employed near the critical point.

To summarize, we have confirmed the localization-delocalization transition in the DQSW model by using the fractal analysis of the wave functions in systems with varying parameters. We find that the size-independent linear relationship of function $v(x)$ persists near the critical point p_c. This behavior not only indicates the exact multifractality of the wave functions at the critical point, but also produces a universal critical singularity spectrum $f_c(\alpha)$ independent of the parameters. Moreover, we find that the transition from the localization to the delocalization in the DQSW systems can also be displayed by drawing the curves of $\alpha_0(p)$ and $\alpha_1(p)$ versus p which cross the reference critical lines at the transition. The present investigations may shed some light on properties of disordered systems with varying effective dimensionality.

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