

Localization-delocalization transition of electron states in a disordered quantum small-world network

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We investigate the localization behavior of electrons in a random lattice that is constructed from a quasi-one-dimensional chain with a large coordinate number Z and rewired bonds, resembling the small-world network proposed recently, but with site-energy disorder and quantum links instead of classical ones. The random rewiring of bonds in the chain with large Z enhances both the topological disorder and the effective dimensionality. From the competition between disorder and dimensionality enhancement a transition from localization to delocalization is found by using the level statistics method. The critical value of the rewiring rate for this transition is determined numerically. We obtain a universal critical integrated distribution of level spacing s in the form $I_{p_c}(s) \propto \exp(-A_c s^\alpha)$, with $A_c \approx 1.50$ and $\alpha \approx 1.0$. This reveals the possible existence of metal-insulator transition in materials with chains as the backbones.

I. INTRODUCTION

The small-world network (SWN) model proposed by Watts and Strogatz¹ has recently attracted much attention since it can describe typical properties of diverse materials ranging from regular lattices to random graphs simultaneously by varying only a single parameter. Most of the previous works have focused on the average minimal distance \bar{l} separating two randomly chosen points that describes how the distance is reduced by the rewiring of the bonds in the network. Several numerical and analytical studies have investigated the crossover behavior,² the scaling properties,³ and the percolation of the dynamic processes⁴ in this model. Although the connection between any two vertices, no matter whether it is a regular link or a “shot-cut,” is treated as a classical one up till now, the model has shown its wide applications on modeling communication networks, disease spreading, power grid, etc. To stimulate out new applications of SWN in condensed matter physics, it is interesting to introduce quantum connections instead of classical ones among vertices and to investigate the properties of electronic states. By rewiring the bonds from a one-dimensional (1D) chain with a large coordinate number, the lattice becomes random and its effective dimension increases. If the diagonal disorder is also included, it becomes a suitable model to probe the localization and delocalization behavior for realistic systems for which the backbones are 1D chains.

The construction of a small-world network starts from a regular 1D chain with a circular boundary condition, in which every site is connected to its Z immediate neighbors. Then every bond starting from a site can be rewired with a probability p , i.e., to be replaced by a new bond from the same site to a randomly chosen site other than one of the Z neighbors. From the geometric point of view, the rewiring procedure introduces the topological disorder to the originally regular 1D lattice but generates many “shot-cut” paths for the moving of particles, causing easier spreading of the

states. At the same time the additional site-energy disorder tends to localize the states. Therefore, there are two competing effects on localization properties of electronic states: one is the localization effect produced by the topological and diagonal disorder; the other is the spreading effect caused by the “shot-cut” links. In fact, such “shot-cut” links eventually lead to the enhancement of the effective dimensionality of systems in the case of large Z . Thus a metal-insulator transition (MIT) can be expected by varying p if the effective dimensionality exceeds 2. The purpose of this paper is to investigate localization properties of electrons in such a disordered quantum small-world (DQSW) model, and to seek for the possible transition between localization and delocalization. We discern the localized and delocalized states from the level statistics method. We determine the transition and obtain a universal critical distribution of level spacing at the critical points, revealing the possible existence of MIT in some soft materials.

The paper is arranged as follows: in Sec. II we describe the structure and basic formalism of the DQSW model; in Sec. III we show numerical results on typical level spacing distributions; we present the scaling of the level statistics for the phase transition in Sec. IV; and we give a brief summary in Sec. V.

II. BASIC FORMALISM

Consider an electron moving in a DQSW network, the tight-binding Hamiltonian of the system 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 ϵ_i is energy level on site i , N is the total number of sites, Z defines the immediate neighboring range $[i - Z/2, i + Z/2]$ of site i , i_R is an arbitrary site outside this range and

subject to the restriction that there is no repeated term in the sum, and t_1 and t_2 are hopping integrals for “original” and “rewired” links, respectively. Here, ϵ_i and $\rho_{i,l}$ are random variables satisfying the distribution probabilities

$$P(\epsilon_i) = \begin{cases} 1/w & \text{if } -w/2 \leq \epsilon_i \leq w/2 \\ 0 & \text{otherwise,} \end{cases} \quad (2)$$

$$P(\rho_{i,l}) = \begin{cases} p & \text{if } \rho_{i,l} = 1 \\ 1-p & \text{if } \rho_{i,l} = 0. \end{cases} \quad (3)$$

Thus w characterizes the degree of on-site disorder as in the Anderson model.⁵

Actually, the present model provides a way to describe the random topological structures in some realistic soft materials. In the case of polymer, the intrachain winding⁶ could serve as a possible rewiring mechanism, and both topological and site-energy disorder could exist. Moreover, the circular boundary condition for a long chain that yields the circle structure of a typical small-world network is also applicable in an analysis of the quasi-1D systems.

III. LEVEL STATISTICS

The Hamiltonian matrix can be diagonalized numerically to yield the single-electron eigenvalue spectrum. It is well known that the levels of the localized and extended states exhibit sharply different level spacing distributions. The localized states have the exponential decay of the space overlapping so that their levels are unrelated. After unfolding^{7,8} the level spacing s obeys Poisson distribution $P_P(s) = \exp(-s)$ when the size of system goes to infinity. Meanwhile the extended states of consecutive energy levels have a large space overlapping, resulting in a correlated energy spectrum with level spacing satisfying Wigner-Dyson (W-D) distribution $P_{W-D}(s) = (\pi/2)s \exp(-\pi s^2/4)$.

In order to obtain a quantitative description, we adopt a variable η to depict the relative deviation of variance $\text{var}(s)$ of level distribution $p(s)$ from that of the W-D distribution:⁹

$$\eta(p, w, Z, N) = \frac{\text{var}(s) - 0.273}{1 - 0.273}, \quad (4)$$

where 0.273 and 1 are the variance of W-D and Poisson distributions, respectively. Thus η can serve as a measure of the deviation of states from the extended states. To suppress the fluctuations in the results we take an ensemble average over 10-100 random configurations. For the sake of simplicity we set t_1 as the energy units. The degree of on-site disorder w varies from 0 to 22, and the rewiring probability p is ranged from 0 to 0.95. In the calculations we take $Z=8$ or 4 and $t_2=1, 0.3$, or 0.1 to check their effect on the localization varying the system size from $N=1200$ to $N=3600$.

In Fig. 1 we show the level spacing distribution of systems with different p reflecting the delocalization effect of the rewiring. It is easily understood from the scaling theory¹⁰ that the states are localized for the system with zero p and finite w because of its 1D nature. Although Fig. 1 only shows the behavior of the system with fixed size, the typical W-D form of the distributions for $p \sim 0.2$ suggests the extended nature of the states. Note that the crossing point $s_0 \approx 2.0$ of

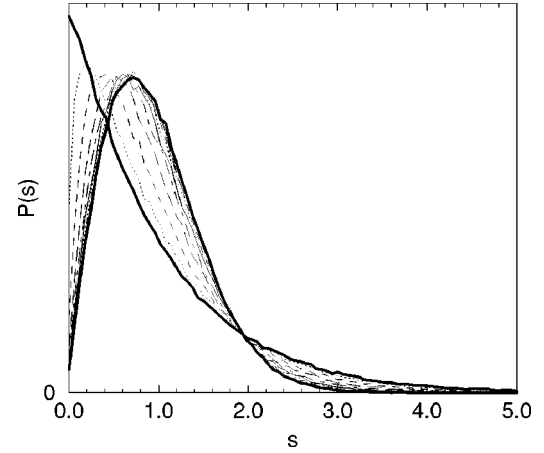


FIG. 1. Level spacing distribution $P(s)$ for system with parameters $N=1600$, $w=16.0$, $Z=8$, and $t_2=1$. t_1 is set to be the energy units. The rewiring probability varies as $p=0, 0.02, 0.04, \dots, 0.20$ for curves from the Poisson-like form to the Wigner-Dyson-like form. The curves cross at the common point $s_0 \approx 2.0$.

the curves is independent of the parameters, suggesting the applicability of the level statistics for the present model.

The values of other parameters also have a crucial effect on the localization behavior of the states. Increasing the coordinate number Z will accelerate the delocalization in increasing p from zero. It is difficult to find the extended states if $Z \leq 4$. The hopping intensity t_2 of the rewired bonds has a similar effect on the localization. The extended states cannot be found if t_2 is too small. The degree of topological disorder is enhanced by decreasing the ratio t_2/t_1 from 1. At this point the DQSW model is essentially different from the classical SWN, in which the properties depend only on the structural parameters. In Fig. 2 we plot the dependence of η on parameters w and p for various system sizes and other choices of Z and t_2 . η varies monotonically with increase of w for all the investigated system sizes, reflecting the trivial localization effect of the on-site disorder as in other models. Although η is certainly near zero for small w , η still in-

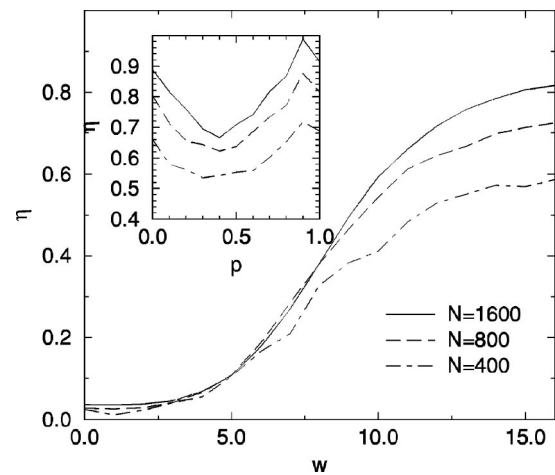


FIG. 2. Scaling variable η as a function of w for systems with $t_2=0.3$, $Z=4$, and $p=0.04$. The size of system is $N=400$ (dotted line), $N=800$ (long-dashed line), and $N=1600$ (solid line). Inset: η vs p curves for systems with $w=8$, $t_2=0.1$, and the same values of other parameters as those in the main panel.

increases by increasing the system size, suggesting the absence of the extended states in the thermodynamical limit. The effect of p is rather nontrivial in the case of $t_2=0.1$ and $Z=4$. Since the rewired links have much weaker hopping strength than the original ones, the p dependence of η is no longer monotonous. It reaches a minimum value η_m at a medium value p_m . When p is small ($p < p_m$), the increase of p creates the long-range hopping paths and causes the states to be more expanded. For large p the hopping strength of the rewired links becomes important and by increasing p more bonds with large hopping intensity are converted to ones with small hopping intensity. This enhances the localization trend and increases the value of η . When p is near 1, the structure approaches the limit of a random graph in which the 1D backbone completely disappears and the original links with $t_1=1$ are almost absent. In this case the increase of long-range paths can result in the decrease of η . All the states are still localized as shown from the N dependence of η . From a comparison of the inset and the main panel, the value of η is increased by decreasing t_2 from 0.3 to 0.1. The p dependence of η is sensitive to the value of t_2 . If $t_2 > 1$, η is monotonically increased with p because by increasing p more bonds are converted from weak hopping to strong hopping.

IV. SCALING BEHAVIOR OF LEVEL SPACING DISTRIBUTION

In a new version of small-world model proposed by Newman and Wattz,⁴ the length scale ξ defined as $\xi=1/p$ for the 1D underlying lattice governs the features of a number of quantities, such as the mean distance of pairs of vertices, the effective dimension D , etc. In their model D is a size-dependent quantity and related to the length scale in the form $D=\ln(pZN)$. In the quantum version of a small-world network, p still plays an important role in determining the localization properties of electrons, although we adopt the structure of the earlier version of the model proposed in 1 and include the diagonal disorder. One can conjecture that by the random rewiring procedure the effective dimension is still related to Z and p , although the relation $D=\ln(pZN)$ may no longer be valid. In this sense for large Z and suitable p the effective dimensionality of DQSW can exceed 2. One could predict the occurrence of MIT in such systems without violating the scaling hypothesis.

In Fig. 3 we plot the p dependence of η varying N . The curves cross at $p_c \sim 0.085$ and $\eta_c = 0.37$. p_c can be regarded as the transition point separating the localization regime ($p < p_c$) and the delocalization regime ($p > p_c$). The w dependence of p_c in $Z=8$ is shown in the inset of Fig. 3. p_c increases with w as can be expected from the trivial effect of w .

It is interesting to investigate the level statistics at the critical points. For this purpose it is more convenient to consider the cumulative level spacing distribution function⁹ $I(s) = \int_s^\infty p(s') ds'$. One has $I_p(s) = \exp(-s)$ and $I_w(s) = \exp(-\pi s^2/4)$ for the Poisson and W-D distributions, respectively. To demonstrate the universal feature of the distribution at the critical points, in Fig. 4 we plot the $-\ln I(s)-s$ curves for parameters in the localization and delocalization regimes and at the critical points. We find that in

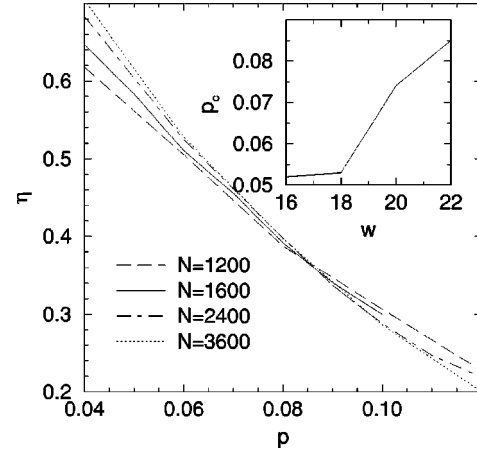


FIG. 3. Scaling variable η as a function of p for systems with $Z=8$, $w=22$, $t_2=1.0$, and various system sizes N . Critical rewiring probability $p_c=0.085$ is determined from the crossing point. Inset: Critical rewiring probability p_c as a function of the on-site disorder w .

the range of $s \geq 0.5$ all the curves corresponding to the critical points for various values of N and w coincide with a common straight line, which can be fitted by

$$I_c(s) \propto \exp(-A_c s^\alpha), \quad (5)$$

with $A_c = 1.50 \pm 0.06$ and $\alpha = 1.0$ independent of the values of w and N . Since $\alpha=1$ the critical distribution $P_c(s)$ is similar to the Poisson distribution in the tail of large s . This feature of the critical distribution at large s has been obtained in the Anderson transition in a system of very large size.¹¹ In the range $s < 0.5$, the curves $-\ln I(s)$ vs s for the critical

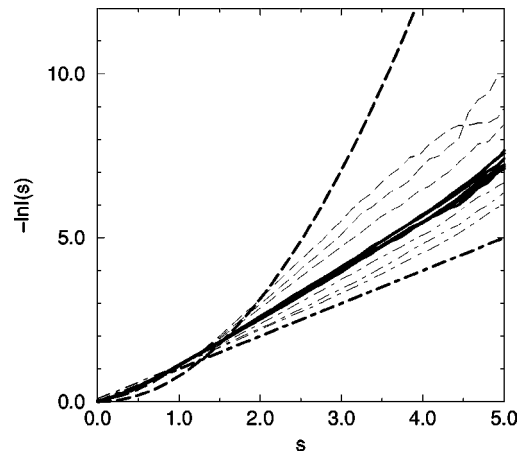


FIG. 4. Logarithmic integrated level spacing distribution $-\ln[I_c(s)]$ at the critical points p_c for systems with different N and w (thick solid curves). The distributions for systems in the noncritical regimes are shown by the thin dashed lines (delocalization regime) and the thin dot-dashed lines (localization regime). Delocalization regime: $N=1200$, $w=18$, $p=0.12$; $N=1600$, $w=18$, $p=0.10$; and $N=1600$, $w=22$, $p=0.20$. Localization regime: $N=1600$, $w=18$, $p=0.03$; $N=1200$, $w=22$, $p=0.02$; and $N=1600$, $w=22$, $p=0.01$. The Poisson and Wigner-Dyson distributions are plotted as references with thick dot-dashed line and thick dashed line, respectively. All the distributions at the critical points for $s > 0.5$ collapse in a common straight line fitted by $-\ln I_c(s) = 1.5s - 1.0$.

points are deviated from the straight line and approach to a function in the form of $\exp(-\pi s^{\alpha_1}/4)$, with $1 < \alpha_1 < 2$. This behavior interpolates between Poisson and W-D distributions. Such a universal form for the critical points provides further evidence for the existence of the transition in the DQSW system.

V. DISCUSSION AND CONCLUSIONS

We have investigated the small-world model from the viewpoint of the quantum Hamiltonian with the primary topological disorder in the network and the additional diagonal disorder. Similar to the cases of earlier works that focus on the classical behavior of this structure, we find that the rewiring procedure with probability p not only introduces the topological disorder, but also enlarges the effective dimensionality of the system. As a result of the competition between these two effects, the system undergoes a metal-insulator phase transition by varying p . By using the method of level statistics, we have determined the w -dependent transition point p_c in the DQSW system. It corresponds to a

transition of the level distribution $P(s)$ from the Poisson-like form to the Wigner-Dyson-like form. The calculated critical point p_c increases by increasing the diagonal disorder w . Moreover, it belongs to a universal sort of phase transition characterized by the critical distribution $\ln I_{p_c}(s) \propto -1.5s$ at large s . The existence of such a transition depends crucially on values of other parameters such as Z and t_2 . When the hopping intensity of rewired bonds t_2 is too small, the disorder effect of the rewiring process becomes dominant and no extended states can be found. Furthermore, the transition usually does not occur if $Z \leq 4$, because in this case the effective dimensionality cannot exceed 2 in the rewiring process.

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