Localization-Delocalization Transition of Electron States in a Disordered Quantum Small World Network

Chen-Ping Zhu\textsuperscript{1,2} and Shi-Jie Xiong \textsuperscript{1}

\textsuperscript{1}National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, People’s Republic of China

\textsuperscript{2}College of Science, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, People’s Republic of China

Abstract

We investigate the localization behavior of electrons in a random lattice which is constructed from a quasi-one-dimensional chain with 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 combined with the finite-size scaling analysis. 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 $I_{pc}(s) \propto \exp(-A_c s^\alpha)$, with $A_c \simeq 1.50$ and $\alpha \simeq 1.0$. This reveals the possible existence of metal-insulator transition in materials with chains as the backbones.

PACS numbers: 73.61.Ph, 05.60.+w, 71.30.+h, 72.90.+y
I. INTRODUCTION

Small-world network (SWN) model proposed by Watts and Strogatz [1] 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 $l$ separating two randomly chosen points which 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 processes [4] in this model. Although the connection between any two vertices, no matter 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, and 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 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 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 moving of particles, causing easier spreading of the states. At the same time the additional site-energy disorder trends 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 combined with the finite-size scaling analysis. 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 section II we describe the structure and basic formalism of the DQSW model; in section III we show numerical results on typical level spacing distributions; we present the scaling analysis of the level statistics for the phase transition in section IV; and we give a brief summary in the last section.

II. BASIC FORMALISM

Consider an electron moving in a DQSW network, the tight-binding Hamiltonian of the system reads

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

$$+ t_2 \rho_{i,l} (|i\rangle \langle i_R| + |i_R\rangle \langle i|)],$$

(1)

where $\epsilon_i$ 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 size $i$, $i_R$ 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, $\epsilon_i$ and $\rho_{i,l}$ are random variables satisfying the distribution probabilities.
\[ P(\varepsilon_i) = \begin{cases} 
1/w, & \text{if } -w/2 \leq \varepsilon_i \leq w/2, \\
0, & \text{otherwise}, 
\end{cases} \]  
\tag{2}

\[ P(\rho_{i,t}) = \begin{cases} 
p, & \text{if } \rho_{i,t} = 1, \\
1 - p, & \text{if } \rho_{i,t} = 0. 
\end{cases} \]  
\tag{3}

Thus, \( w \) characterizes the degree of on-site disorder as in the Anderson model \cite{Anderson67} and \( p \) is the probability of a bond in the immediate neighboring range to be broken and rewired. By increasing \( p \) the number of irregular bonds, which are also “short-cut” paths for the motion of electrons, is increased, leading to the enhancement of both the degree of topological disorder and the effective dimensionality.

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 winding \cite{metrical} could serve as possible rewiring mechanism, and both topological and site-energy disorder could exist. Moreover, the circular boundary condition for a long chain which yields the circle structure of a typical small-world network is also applicable in analysis of the quasi-1D systems.

### III. LEVEL STATISTICS

The Hamiltonian matrix can be diagonalized numerically to yield 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 \cite{Gaussian, Wigner} 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 large space overlapping, resulting in a correlated energy spectrum with level spacing satisfying Wigner-Dyson (W-D) distribution \( P_{W-D}(s) = \frac{\pi}{2} s \exp(-\pi s^2/4). \)
A DQSW system is characterized by the following parameters: the degree of diagonal disorder \( w \), the rewiring probability \( p \), the coordination number of the original 1D chain \( Z \), the ratio of the rewired hopping integral to the original one \( t_2/t_1 \), and the size of system \( N \).

If \( w \neq 0 \) and \( p = 0 \), it is simply a 1D disordered model with circular boundary condition and all the states are localized. In this case \( P(s) \) exhibits Poisson distribution. By increasing \( p \), the degree of the topological disorder increases but the probability for an electron to tunnel to farther sites is also enhanced, leading to the competition of two opposite effects for the localization. The including of the on-site disorder provides another mechanism of changing the balance of the competition. In order to obtain a quantitative description of the resultant effect of the competition, we adopt a scaling variable \( \eta \) to depict the relative deviation of variance \( \text{var}(s) \) of level distribution \( p(s) \) from that of the W-D distribution. The variance is defined as

\[
\text{var}(s) = \langle s^2 \rangle - \langle s \rangle^2,
\]

and the scaling function is

\[
\eta(p, w, Z, N) = \frac{\text{var}(s) - 0.273}{1 - 0.273},
\]

where 0.273 and 1 are the standard variance of W-D and Poisson distributions, respectively. Thus \( \eta \) can serve as a measure of the deviation of states from the extended states. From this definition we can calculate \( p \) and \( w \) dependence of \( \eta \) for given values of other parameters.

To suppress the fluctuations in the results we take 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. Meanwhile the scaling analysis is carried out by varying the system size from \( N = 1200 \) to \( N = 3600 \).

In Fig. 1 we show the level spacing distribution of systems with different rewiring probability and fixed values of \( w, Z, t_2 \) and \( N \). By increasing the rewiring probability \( p \)
from zero $P(s)$ varies from Poisson-like to Wigner-Dyson-like for a finite $w$, reflecting the delocalization effect of the rewiring. It is easily understood from the scaling theory [10] that the states are localized for system with zero $p$ and finite $w$ because of its 1D nature. By increasing $p$ both the degree of topological disorder and the effective dimensionality of the system are enhanced. The results of Fig. 1 indicate that the latter is dominant for $Z = 8$, $t_2 = 1$ and the adopted range of $p$. The appearance of the extended states is possible if the effective dimensionality exceeds 2. Although Fig. 1 only shows the behavior of system with fixed size, the typical W-D form of the distributions for $p \sim 0.2$ suggests the extended nature of the states. We will carry out the scaling analysis to check the existence of MIT. Note that the crossing point $s_0 \simeq 2.0$ of the curves is independent of the parameters, suggesting the applicability of the level statistics for the present model.

The values of other parameters, such as $Z$ and $t_2$, also have crucial effect on the localization behavior of the states. Generally speaking, increasing the coordinate number $Z$ will accelerate the tendency of delocalization in increasing $p$ from zero. It is difficult to find the extended states if $Z \leq 4$. The value of $t_2$, the hopping intensity of the rewired bonds, has similar effect on the localization effect of the states. The extended states can not 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. Thus, in increasing $p$ the effect of enlarging effective dimensionality may be cancelled by the increase of the disorder. 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 scaling variable $\eta$ on parameters $w$ and $p$ for various system sizes and other choices of $Z$ and $t_2$. It can be seen from the main panel that $\eta$ 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 $\eta$ is certainly near zero for small $w$, $\eta$ still decreases by increasing the system size, suggesting the absence of the extended states in the thermodynamical limit. This implies that for $Z = 4$, $t_2 = 0.3$ and $p = 0.04$, the effective dimensionality could not exceed 2. From the inset it can be seen that the effect of $p$ is rather nontrivial in the case of $t_2 = 0.1$ and $Z = 4$. 

6
Since the rewired links have much weaker hopping strength than the original ones, the $p$ dependence of $\eta$ is no longer monotonous. It first decreases with $p$ and reaches a minimum value $\eta_m$ at a medium value $p_m$, then increases and finally drop down again near $p = 1$. This behavior is not changed by changing the system size. 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 $\eta$. When $p$ is near 1, the structure approaches to 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 increase of $\eta$. All the states are still localized as shown from the $N$ dependence of $\eta$. From comparison of the inset and the main panel, the value of $\eta$ is increased by decreasing $t_2$ from 0.3 to 0.1. It should be stressed that the $p$ dependence of $\eta$ is sensitive to the value of $t_2$. If $t_2 > 1$ $\eta$ 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, the length scale $\xi$ defined as $\xi = \frac{1}{p}$ 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 $D = \log(pZN)$. In the quantum version of small-world network, $p$ still plays an important role in determine the localization properties of electrons, although we adopt the structure of the earlier version of the model proposed in 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 $D = \log(pZN)$ 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 $\eta$ for systems with varying size ($N = 1200, 1600, 2400$ and $3600$) and with parameters $t_1 = t_2 = 1, Z = 8$ and $w = 22$. The curves corresponding to different system sizes are crossed at point $p_c \sim 0.085$ for which $\eta(p)$ is size-independent and equal to $\eta_c = 0.37$. $p_c$ can be regarded as the transition point separating the localization regime ($p < p_c$) and delocalization regime ($p > p_c$). We also find that this transition can occur in a range of $w$. 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 $w$.

The values of $\eta$ shown in Fig. 3 as a function of $p$ and $L$ can be fitted with a one-parameter scaling function

$$\eta(L, p) = f(L/\xi(p)), \quad (6)$$

where $\xi(p)$ can be regarded as the localization length in the localized regime and the correlation length in the delocalized regime. We set up the value of $\xi(p)$ in such a way that all the $\eta(L, p) - L/\xi(p)$ curves from the data of Fig. 3 can collapse in a common curve representing the function $f(L/\xi(p))$. In the inset of Fig. 4 we plot this function. It can be seen that the curve consists of two branches: the upper branch corresponds to the localization regime ($p < p_c$) and the lower branch stands for the delocalization regime ($p > p_c$). The value of $\xi$ is singular at the transition point $p_c$. This singularity can be expressed by a power law with exponent $\nu$

$$\xi(p) = \xi_0 |p - p_c|^{-\nu}, \quad (7)$$

where $\xi_0$ is a constant. By fitting the data we obtain that the exponent is equal to $\nu = 0.92 \pm 0.15$.

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 function defined in the form $[9]$ $I(s) = \int_{s'}^{\infty} p(s')ds'$. From this definition 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 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 fitted by

\[ I_c(s) \propto \exp(-A_c s^\alpha) \]  

with coefficient \(A_c = 1.50 \pm 0.06\) and exponent \(\alpha = 1.0\) 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 system of very large size [11]. In the range \(s < 0.5\), the curves \(-\ln I(s)\)-s for the critical points is deviated from the straight line and approaches to a function of the form of Eq. (8) but with \(\alpha\) greater than 1. This is a behavior that interpolates between poisson and W-D distributions. Such a universal form for the critical points provides the further evidence for the existence of the transition in the DQSW system. Moreover, it is a successful practice of the new method using the level statistics combined with the finite size scaling analysis proposed in Ref. [9] to determine the localization-delocalization transition in systems with complicated structures.

**V. DISCUSSION AND CONCLUSIONS**

We have investigated the small-world model in the viewpoint of quantum Hamiltonian with the primary topological disorder in the network and the additional diagonal disorder. Similarly to the case of the earlier works which 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 combined with the finite
size scaling analysis, 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. For this transition a two-branch scaling function is obtained. The calculated critical point $p_c$ increases with 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 can not exceed 2 in the rewiring process.

ACKNOWLEDGMENTS

We would like to thank S.N. Evangelou for useful discussion. This work was supported by National Foundation of Natural Science in China Grant No. 69876020 and by the China State Key Projects of Basic Research (G1999064509).
REFERENCES

[1] Duncan J. Watts and Steven H. Strrogatz, Nature 393, 440, (1998).
[2] M. Barthelemy and L.A.N. Amaral, Phys. Rev. Lett 82, 3180 (1999).
[3] R.V. Kulkani, E. Almmas and D. Stroud, cond-mat/9908210.
[4] M.E.J. Newman and D.J. Wattz Phys. Rev. E 60, 6263 (1999).
[5] P.W. Anderson, Phys. Rev. 109, 1492 (1958).
[6] S.J. Xiong and S.N. Evangelou, Phys. Rev. B 52, R13079 (1995).
[7] E. Hofstatter and M. Schreiber, Phys. Rev. B 48, 16979 (1993).
[8] O. Bohigos, M. J. Giannoni, and C. Schmit, Phys. Rev. Lett. 52, 1 (1984).
[9] E. Cuevas, Phys. Rev. Lett. 83, 140 (1999).
[10] E. Abrahams, P.W. Anderson, D.C. Licciardello, and T.V. Ramkrishnan, Phys. Rev. Lett. 42, 673 (1979).
[11] I.Kh. Zharekeshev and B. Kramer, Phys. Rev. Lett. 79, 717 (1997).

Figure Captions

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 successively as $p = 0, 0.02, 0.04, 0.06, 0.08, 0.10, 0.12, 0.14, 0.16, 0.18$, and $0.20$ for curves from the Wigner-Dyson-like form to the Poisson-like form. The curves are crossed at the common point $s_0 \simeq 2.0$.

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

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 non-critical 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 $-\ln I_c(s) = 1.5s - 1.0$. Inset: One-parameter scaling function $\eta(L, p)$ versus $L/\xi$. 
fig. 1
fig. 2
fig.3

$p$ vs $\eta$ for different values of $N$:
- $N=1200$
- $N=1600$
- $N=2400$
- $N=3600$

$\rho_c$ vs $w$ in the inset graph.
fig. 4

\[ -\ln I(s) \]

\[ \frac{L}{\xi} \text{ (arb. units)} \]

\[ \eta(p,N) \]

\[ 0 \quad 1 \quad 10 \quad 100 \]