Coherent exciton transport on scale-free networks

X P Xu$^{1,2,3}$ and F Liu$^1$

$^1$ Institute of Particle Physics, HuaZhong Normal University, Wuhan 430079, People’s Republic of China
$^2$ Institute of High Energy Physics, Chinese Academy of Science, Beijing 100049, People’s Republic of China
E-mail: xuxp@mail.ihep.ac.cn

New Journal of Physics 10 (2008) 123012 (9pp)
Received 12 August 2008
Published 9 December 2008
Online at http://www.njp.org/
doi:10.1088/1367-2630/10/12/123012

Abstract. The coherent exciton transport on a class of deterministic and random scale-free networks (DSFNs and RSFNs) generated by simple rules is studied in this paper. The coherent exciton dynamics is modeled by continuous-time quantum walks, and we calculate the transition probabilities between two nodes of the networks. We find that the transport depends on the initial nodes of the excitation. For DSFNs, the probabilities of finding the excitation at the initial central nodes are nearly periodic, in contrast to the flat behavior found for RSFNs. In the long time limit, the transition probabilities on DSFNs show characteristic patterns with identical values. For RSFNs, we find that the excitation is most likely to be found at the initial nodes with high connectivity. All these features of quantum transport are significantly different from those of the classical transport modeled by continuous-time random walks.

$^3$ Author to whom any correspondence should be addressed.

New Journal of Physics 10 (2008) 123012
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Many social, communication, biological and chemical systems in Nature can be properly described as complex networks [1]. A universal feature of these complex networks is that they have a scale-free structure characterized by the power-law degree distributions \( P(k) \sim k^{-\gamma} \), with the exponent \( \gamma \) usually in the range \( 2 < \gamma < 3 \) [2]. The ubiquity of scale-free (SF) networks in various fields of science has led to many exciting insights into the fundamental principles governing such systems [3, 4]. It has been shown that physical and dynamical processes, such as cascading failures [5], epidemic spreadsings [6], synchronization [7] and quantum transport [8]–[10], are strongly influenced by the structure of the underlying network. The problem of quantum transport modeled by random walks has been widely studied and is relevant to many distinct fields, such as polymer physics, solid-state physics, biological physics and quantum computation [11, 12]. The behavior of quantum transport on networks differs from that of the classical random walks in several striking ways, due to the fact that quantum walks exhibit interference patterns, whereas the classical random walks do not. Previous studies on quantum transport have focused on simple structures, such as a line [13], a cycle [14], a hypercube [15], a Cayley tree [16], dendrimers [17] and other regular networks with a simple topology [18, 19], and there is no published study on quantum transport on SF networks.

In this paper, we study quantum exciton transport on a class of deterministic and random SF networks (DSFNs and RSFNs), which are generated by the following four SF models:

- **Model I** [20, 21]: at the initial generation \( v = 0 \), the network is composed of two connected nodes. At the subsequent generation, a pair of new nodes are attached to the ends of each edge of the existing graph (see figure 1).
- **Model II** [21, 22]: at the initial generation \( v = 0 \), the network is composed of three fully connected nodes. At the subsequent generation, each edge of the present graph generates a new node and connects to both nodes of the edge (see figure 1).
- **Model III** [23]: at the initial configuration \( T = 2 \), the network is composed of two connected nodes; at the subsequent step, a new node is created and connected to the previous nodes according to the linear preferential attachment [24].
- **Model IV** [25]: initially when \( T = 3 \), the network is composed of three fully connected nodes. At the subsequent step, a new node is added and connected to both ends of a randomly chosen edge by two links.

Models I and III generate networks with a tree structure, and the networks of models II and IV have a loop structure; we expect that these network characteristics will have some impact on the properties of the coherent exciton transport taking place on them.

The coherent exciton transport on a connected network is modeled by continuous-time quantum walks (CTQWs), which are obtained by replacing the Hamiltonian of the system by the classical transfer matrix, i.e. \( H = -T \) [16, 19]. The transfer matrix \( T \) is related to the Laplace matrix \( A \) by \( T = -A \) [17]–[19]. The Laplace matrix \( A \) has nondiagonal elements \( A_{ij} \), which are equal to \(-1\) if nodes \( i \) and \( j \) are connected and are 0 otherwise. The diagonal elements \( A_{ii} \) are equal to the degree of node \( i \), i.e. \( A_{ii} = k_i \). The states \( |j\rangle \) endowed with node \( j \) of the network form a complete, orthonormalized basis set, which spans the whole accessible Hilbert space. The classical and quantum transition probabilities to go from the state \( |j\rangle \) at time 0 to the state \( |k\rangle \) at time \( t \) are given by \( p_{k,j}(t) = \langle k|e^{-itA}|j\rangle \) and \( \pi_{k,j}(t) = |\langle k|e^{-itH}|j\rangle|^2 \) [17, 19], respectively. Using \( E_n \) and \( |q_n\rangle \) to represent the \( n \)th eigenvalue and orthonormalized
Figure 1. Deterministic networks generated by models I (a) and II (b) in three generations. The nodes of both the graphs are classified into eight groups according to the affiliated relationship in the generation. The symbol of the group indicates the associated relation between the present group and the previous group. For instance, $G_{2,0}$ represents the cluster of nodes that are connected to the nodes of group $G_0$ in the second generation.

| Generation | Graph (a)            | Graph (b)            |
|------------|----------------------|----------------------|
| $v=0$      | $G_0$: 1,2           | $G_0$: 1-3           |
| $v=1$      | $G_{1,0}$: 3,4       | $G_{1,0}$: 4-6       |
| $v=2$      | $G_{2,0}$: 5-8       | $G_{2,0}$: 7-9       |
|            | $G_{2,1}$: 9,10      | $G_{2,1}$: 10-15     |
| $v=3$      | $G_{3,0}$: 11-18     | $G_{3,0}$: 16-18     |
|            | $G_{3,1}$: 19-22     | $G_{3,1}$: 19-24     |
|            | $G_{3,20}$: 23-26    | $G_{3,20}$: 25-30    |
|            | $G_{3,21}$: 27,28    | $G_{3,21}$: 31-42    |

The eigenvector of $H$, the classical and quantum transition probabilities between two nodes can be written as

$$p_{k,j}(t) = \sum_n e^{-t E_n} \langle k|q_n\rangle \langle q_n|j\rangle,$$

$$\pi_{k,j}(t) = |\alpha_{k,j}(t)|^2 = \sum_n e^{-i t E_n} \langle k|q_n\rangle \langle q_n|j\rangle|^2.$$

Generally, to get $p_{k,j}(t)$ and $\pi_{k,j}(t)$, all the eigenvalues and eigenvectors of the transfer operator and Hamiltonian are required. Here, we consider transition probabilities on SF networks with particular attention to the probabilities of finding the excitation at the initial node, namely the return probabilities, $p_{j,j}(t)$ and $\pi_{j,j}(t)$. The eigenvalues and eigenvectors are obtained by numerically diagonalizing the Hamiltonian $H$ by using a standard software package, Mathematica 5.0.

First, we consider $p_{j,j}(t)$ and $\pi_{j,j}(t)$ on DSFNs obtained in three generations. The advantages of DSFNs enable us to neglect the statistical uncertainty of the network structure. The nodes of the resulting graphs are classified into eight groups as indicated in figure 1. Figure 2 shows $p_{j,j}(t)$ and $\pi_{j,j}(t)$ for nodes of different groups. For nodes of the initial generation $v = 0$, i.e. $j \in G_0$, $\pi_{j,j}(t)$ shows regular oscillations. It is found that the period for networks produced by model I is larger than that for networks produced by model II (compare panels (1a) and (1b) of figure 2). Such a phenomenon is more visible for groups created in the initial generation.
Figure 2. Time evolution of return probabilities on DSFNs generated by model I (column (a)) and model II (column (b)) in three generations. The size of the two graphs is $N = 28$ (model I) and $N = 42$ (model II), respectively. We show the return probabilities for nodes of the eight groups classified in figure 1. Row 1: $\pi_{j,j}(t)$ versus $t$ for $j \in G_0$. Row 2: $\pi_{j,j}(t)$ for $j \in G_{1,0}$. Row 3: $\pi_{j,j}(t)$ for nodes generated in the second generation, i.e. $j \in G_{2,0}$ and $G_{2,1}$. Row 4: $\pi_{j,j}(t)$ for nodes generated in the third generation, i.e. $j \in G_{3,0}$, $G_{3,1}$, $G_{3,20}$ and $G_{3,21}$. Row 5: Classical $p_{j,j}(t)$ for nodes of all the groups.

first generation $v = 1$ ($j \in G_{1,0}$). As the generation increases, the oscillation becomes irregular (see the plots in the third and fourth rows of figure 2). The return probability is nearly periodic at the central node and becomes irregular at the periphery. The periodic oscillation of $\pi_{j,j}(t)$
Figure 3. Ensemble averaged return probabilities $\langle \pi_{j,j}(t) \rangle$ and $\langle p_{j,j}(t) \rangle$ for nodes added at times $T = 1, T = 10$ and $T = 100$ on RSFNs generated by model III (a) and model IV (b). The size of all the networks is $N = 100$ and all the curves are averaged over 100 different realizations.

suggests that there are partial revivals of the initial state when the initial excitation starts at the central node. This revival of the initial probability resembles results obtained for continuous and discrete quantum carpets [26]–[28]. The classical return probabilities $p_{j,j}(t)$ for different groups are shown in the last row of figure 2. As we can see, $p_{j,j}(t)$ for the eight groups differs from each other. If the excitation starts at the central nodes ($j \in G_0$), the equipartition probability $1/N$ is reached much faster than when starting at other nodes. For groups of the same generation, the classical return probability for nodes generated by early generation reach equipartition $1/N$ very quickly (compare the curves of $p_{j,j}(t)$ for $j \in G_{3,0}, G_{3,1}, G_{3,20}$ and $G_{3,21}$). A similar behavior of $p_{j,j}(t)$ and $\pi_{j,j}(t)$ is also found for networks of higher generations.

Next, we consider $p_{j,j}(t)$ and $\pi_{j,j}(t)$ on RSFNs of size $N = 100$ produced by models III and IV. In order to reduce the statistical fluctuation of the network structure, we average the return probabilities over distinct single networks. Figure 3 shows the ensemble averaged return probabilities $\langle \pi_{j,j}(t) \rangle$ and $\langle p_{j,j}(t) \rangle$ for nodes added at time (step) $T = 1, T = 10$ and $T = 100$. It is found that $\langle \pi_{j,j}(t) \rangle$ does not oscillate but retains a steady value around the long time averages. The steady value depends on the initial nodes where the excitation starts. We find that $\langle \pi_{j,j}(t) \rangle$ has a larger steady value for nodes added at earlier times. This effect is more visible for the graphs generated by model IV. The classical return probabilities $\langle p_{j,j}(t) \rangle$ ($j = 1, 10$ and 100) converge to the equipartitioned probability $1/N = 0.01$, and the excitation starting at old nodes reaches equipartition faster than that starting at subsequent nodes. Furthermore, equipartition is reached much faster on networks of model IV than on those of model III. Here, the difference in $\langle \pi_{j,j}(t) \rangle$ on RSFNs and DSFNs is remarkable. The regular oscillation on DSFNs can be regarded as a natural consequence of the symmetry of the network structure. However, for RSFNs such a topological symmetry does not exist, resulting in a rather flat behavior of $\langle \pi_{j,j}(t) \rangle$. 

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Now we consider the long-time averages of the transition probabilities $p_{j,k}(t)$ and $\pi_{j,k}(t)$. On finite networks, the transition probability converges to a certain value. Classically, this value is equal to the equal-partitioned probability $1/N$. However, the quantum transport does not lead to equipartition. For DSFNs, the long-time average of $\pi_{j,k}(t)$ is

$$
\chi_{k,j} = \lim_{T \to \infty} \frac{1}{T} \int_0^T \pi_{k,j}(t)dt
$$

$$
= \sum_{n,l} \delta(E_n - E_l)\langle k|q_n\rangle\langle q_n|j\rangle\langle j|q_l\rangle\langle q_l|k\rangle,
$$

where $\delta(E_n - E_l) = 1$ if $E_n = E_l$ and $\delta(E_n - E_l) = 0$ otherwise [17, 19]. Some eigenvalues of $H$ may be degenerate, so the sum in the equation contains terms belonging to different eigenstates. Here, we calculate the limiting transition probabilities $\chi_{k,j}$ according to this equation. For RSFNs, we calculate the limiting probabilities for each single network and average the probabilities over different network realizations.

Figure 4 shows the contour plot of $\chi_{k,j}$ and its ensemble averages $\langle \chi_{k,j} \rangle$ on SF networks. For DSFNs of size $N = 28$ and $N = 42$ produced by models I and II in three generations, there are high return probabilities $\chi_{j,j}$ (see the diagonal in figures 4(a) and (b)). Specifically, when the initial excitation starts at the most connected nodes, there is a relatively large probability to find the excitation at the initial node. If the excitation starts at the nodes of group $G_0$ ($j \in G_0$), $\chi_{j,j}$ has a large value of 0.373 and 0.491 for networks of models I and II, respectively. Except for the large return probabilities at highly connected nodes, there are also large values of $\chi_{j,j}$ for the outermost nodes of the group $G_{1.0}$. For the specific graphs in figure 1, when the excitation starts at the nodes of the group $G_{3.0}$, $\chi_{j,j}$ is equal to 0.571 and 0.486 for the two models, respectively. For groups in the same generation, the values of $\chi_{j,j}$ are different. We find that $\chi_{j,j}$ for groups connected to old groups is larger than that for clusters connected to subsequent groups, i.e. $\chi_{j,j} (j \in G_{3.0}) > \chi_{j,j} (j \in G_{3.10}) > \chi_{j,j} (j \in G_{3.20}) > \chi_{j,j} (j \in G_{3.21})$.

Another interesting feature of the limiting probabilities is that the two different nodes, $k$ and $l$, may have the same transition probability, i.e. $\chi_{k,j} = \chi_{l,j}$. Concretely, for networks generated by model I with a tree structure, we further divide groups $G_{2.0}$, $G_{3.0}$, $G_{3.1}$, and $G_{3.20}$ into two subgroups by diminution of labeled numbers. We find that $\chi_{k,j} (k \neq j)$ has the same value if nodes $k$ and $l$ belong to the same subgroups. If the subgroups (or group) only have two different nodes, $k$ and $j$, the transition probability $\chi_{k,j}$ is equal to the return probability $\chi_{j,j}$ (see the black squares of the diagonal in figure 4(a)). In the case of the two nodes, $k$ and $j$, belonging to two different groups, the values of $\chi_{k,j}$ are equal (see the square regions of the non-diagonal in figure 4(a)). However, this is not true for the transition probabilities between the groups $G_{2.0}$ and $G_{3.20}$; the values of $\chi_{k,j}$ are equal for the nodes of the subgraphs of these two groups (see the region $5 \leq j \leq 9$, $22 \leq k \leq 25$ in the figure). For networks generated by model II with a loop structure, the transition probabilities $\chi_{k,j}$ can also have the same value but the situation is different. If the groups only contain three different nodes, the transition probabilities $\chi_{k,j} (k \neq j)$ between two nodes of the same group have the same value (see figure 4(b)). When the groups contain more nodes, the transition probabilities $\chi_{k,j}$ and $\chi_{l,j}$ of the same group are identical for some special nodes labeled $k$ and $l$, which depends on the initially excited node, namely, $j$. For instance, if the excitation starts at node 10 in figure 1, the transition probabilities $\chi_{12,10}$ and $\chi_{14,10}$ are equal; if the excitation starts at node 31, $\chi_{35,31}$ and $\chi_{39,31}$ have the same value. Other than the identical values of the transition probabilities for nodes of the same group, we also find...
Figure 4. Contour plot of the long-time averaged transition probabilities $\langle \chi_{k,j} \rangle$ on DSFNs ((a) and (b)) and RSFNs ((c) and (d)). The DSFNs are produced by models I and II in three generations and the nodes are labeled with the numbers in figure 1. The RSFNs are generated by models III and IV and the network size is 100. The nodes are labeled according to the time when the nodes are added (created) in the growth process, i.e. node $j$ is added at time $j$. The values of $\langle \chi_{k,j} \rangle$ are averaged over 100 distinct realizations. The color maps are chosen to be the same for all the plots; the dark regions denote large values of $\langle \chi_{k,j} \rangle$ and the bright regions denote low values of $\langle \chi_{k,j} \rangle$.

equal values of the transition probabilities for nodes of different groups. This situation is more complex and requires further study.

The limiting transition probabilities $\langle \chi_{k,j} \rangle$ for RSFNs of $N = 100$ is shown in figures 4(c) and (d). As we can see, the excitation is most likely to be found at the initial nodes (see the diagonals of the plots). Compared with the return probabilities, $\langle \chi_{j,j} \rangle$ and $\langle \chi_{k,j} \rangle$ ($k \neq j$) are small at the left top (or right bottom) corner. This suggests that the transport between high-degree and low-degree nodes is ineffective.

In addition, we find that the return probabilities are not uniform and are dependent on the initially excited nodes. To reveal the general relationship between the average return
Figure 5. The vertex averaged return probability $\bar{\chi}(k)$ versus $k$ for DSFNs generated by model I (a) and model II (b) in six generations. The network size is $N = 730$ and $N = 1095$, respectively. (c) and (d) The average return probability $\langle \bar{\chi}(k) \rangle$ versus $k$ for RSFNs generated by models III and IV. The values of $k$ are logarithmically binned and the network size is $N = 1000$. The errors in the plots are given by the standard deviation of the distinct values of the return probabilities.

probabilities and the degrees, we plot the vertex averaged return probability $\bar{\chi}(k)$ against the degree $k$ for DSFNs generated by models I and II in six generations (see figures 5(a) and (b)). We find that there is a large fluctuation of $\bar{\chi}(k)$ for small values of $k$ (see the large error bars in the plots). This is because $\chi_{i,j}$ have diverse values for different nodes of the same $k$. For RSFNs, we show the average return probability $\langle \bar{\chi}(k) \rangle$ plotted against $k$ in figures 5(c) and (d). The RSFNs are of size $N = 1000$ and are generated by model III (figure 5(c)) and model IV (figure 5(d)). The $k$-axis is logarithmically binned and the data points and error bars are obtained from 100 different realizations of the models. As we can see, there is a large fluctuation of $\langle \bar{\chi}(k) \rangle$ for a wide range of $k$. Except for the case $k = 1$ (figure 5(c)), $\langle \bar{\chi}(k) \rangle$ increases as $k$ grows. This indicates that the excitation is most likely to be found at the initial nodes with high connectivity.

In summary, we have studied coherent exciton transport modeled by QTQWs on a class of DSFNs and RSFNs. The quantum transport exhibits a very distinct behavior compared with the classical random walks. We find that the space-time structures of quantum transport are different on DSFNs and RSFNs: when the excitation starts at the central nodes, the time evolution of the return probability for DSFNs shows nearly periodic oscillations, in contrast to a steady behavior found for RSFNs. In the long time limit, the quantum mechanical transition probabilities on DSFNs show characteristic patterns with identical values. Finally, we find that the excitation is most likely to be found at the initial nodes with high connectivity. Such a dynamical correlation with the network structure is more notable on RSFNs than on DSFNs. The large difference of

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quantum transport on DSFNs and RSFNs is a natural consequence of the distinct topological symmetry and hierarchy of the network structure. We hope that this work sheds some light on quantum mechanical processes on SF networks, and may be a first step toward the study of quantum transport on complex networks.

Acknowledgments

We acknowledge helpful discussions with Prof. Alexander Blumen of University of Freiburg. This work is supported by the National Natural Science Foundation of China under projects 10575042 and 10775058 and the MOE of China under contract number IRT0624 (CCNU).

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