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Continuous-time quantum walks on Erdös–Rényi networks

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ABSTRACT

We study the coherent exciton transport of continuous-time quantum walks (CTQWs) on Erdös–Rényi networks. We numerically investigate the transition probability between two nodes of the networks, and compare the classical and quantum transport efficiency on networks of different connectivity. In the long time limiting, we find that there is a high probability to find the exciton at the initial node. We also study how the network parameters affect such high return probability.

1. Introduction

During the last few years, the coherent exciton dynamics in quantum system has been extensively studied by both experimental and theoretical methods [1,2]. The dynamical behavior of such process depends on the underlying structure of the system under study. Most of previous studies on coherent exciton dynamics are based on simple structures, for example, the line [3,4], cycles [5,6], hypercube [7], Cayley tree [8], dendrimers [9], polymers [10] and other regular networks with simple topology. To the best of our knowledge, the dynamics of exciton on random network has not received much attention [11].

In this Letter, we consider the coherent exciton transport on random networks of Erdös–Rényi (ER). The coherent exciton dynamics is modeled by continuous-time quantum walks (CTQWs), which is a quantum version of the classical random walk and widely studied by various researchers to describe the relaxation processes in complex systems [12,13]. In the mathematical literature, the ER random network is defined as follows [14,15]: Starting with N disconnected nodes, every pair of nodes is connected with probability p $(0 < p < 1)$ and multiple connections are prohibited. The ER random network is one of the oldest and best studied models of networks, and possesses the considerable advantage of being exactly solvable for many of its average properties in the limit of large network size [16]. For instance, one interesting feature, which was demonstrated in their original papers, is that the model shows a phase transition with increasing p at which a giant component forms [16,17]. An alternative and equivalent representation of the ER random graph is to express the graph not in terms of p but in terms of the average degree $\bar{k}$ of the nodes, which is related to the connection probability p as: $\bar{k} = p(N-1) \approx pN$, where the last approximate equality is hold for large N.

In the limit of large network, the degrees of ER random network follow a Poisson distribution peaked at the average degree $\bar{k}$. In order to contrast the resemblance and difference of the transport dynamics on networks with the same average degree, we consider the coherent exciton transport on a configuration model of random networks in which the degree k of each node equals to the average degree $\bar{k}$ ($\bar{k} \in$ *Integers*) of the Erdös–Rényi networks. The method for generating the graph is as follows [18]: one assigns each node $\bar{k}$ ($\bar{k} \in$ *Integers*) stubs—ends of edges emerging from the nodes, and then one chooses pairs of these stubs uniformly at random and joins them together to make complete

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edges. When all stubs have been used up, the resulting graph is a random member of the ensemble of graphs with the equal degree [16,18]. The configuration model of random networks can also be implemented by using the edge-interchanging algorithm, which randomly interchange two existing edges while keep the degree sequence unchanged [19,20]. The configuration model is one of the most successful algorithms proposed for network formation, and has been extensively used as a null model in contraposition to real networks with the same degree distribution in biology, robustness, epidemics spreading and other dynamical processes taking place on complex networks [19,21,22]. Here, we adopt this idea to compare the transport behavior on the two network models. As we will show, although the ensembles of ER model and configuration model have the same average number of connections, the transport dynamics on the two network models are different.

The Letter is structured as follows. In the next section, we briefly review the classical and quantum transport on networks presented in Refs. [23,24]. In Section 3 we study the time evolution of the ensemble averaged return probability on ER networks with different parameters. Section 4 presents the efficiencies of the classical and quantum-mechanical transport, and try to reveal how the network parameters affect the transport efficiency. In Section 5, we consider the distribution of the long time averaged transition probabilities, and explore how the average return probability is related to network parameters. In Section 6, we consider the transport dynamics on extremely connected networks. Conclusions and discussions are given in the last part, Section 7.

2. Transport on networks

The coherent exciton dynamics on a connected network is modeled by the continuous-time quantum walks (CTQWs), which is obtained by replacing the Hamiltonian of the system by the classical transfer matrix, $H = -T$ [25]. The transfer matrix T relates to the Laplace matrix by $T = -\gamma A$ [8]. Here, for the sake of simplicity, we assume the transmission rate γ for all connections equals to 1. The Laplace matrix A has nondiagonal elements A_{ij} equal to -1 if nodes i and j are connected and 0 otherwise. The diagonal elements A_{ii} equal to the number of total links connected to node i, i.e., A_{ii} equals to the degree of node i. The states $|j\rangle$ endowed with the nodes j of the network form a complete, orthonormalized basis set, which span the whole accessible Hilbert space, i.e., $\sum_k |k\rangle\langle k| = 1$, $\langle k|j\rangle = \delta_{kj}$. The transport processes are governed by the master equation or Schrödinger equation [8]. The classical and quantum-mechanical transition probabilities to go from the state $|j\rangle$ at time 0 to the state $|k\rangle$ at time t are given by $p_{k,j}(t) = \langle k|e^{-tA}|j\rangle$ and $\pi_{k,j}(t) = |\alpha_{k,j}(t)|^2 = |\langle k|e^{-itH}|j\rangle|^2$ [8], respectively. Generally speaking, to calculate the transition probabilities, all the eigenvalues and eigenvectors of the transfer operator and Hamiltonian are required. We use E_n to represent the nth eigenvalue of H and denote the orthonormalized eigenstate of Hamiltonian by $|q_n\rangle$, such that $\sum_n |q_n\rangle\langle q_n| = 1$. The classical and quantum transition probabilities between two nodes can be written as

$$p_{k,j}(t) = \sum_n e^{-tE_n}\langle k|q_n\rangle\langle q_n|j\rangle, \tag{1}$$

and

$$\pi_{k,j}(t) = \left|\alpha_{k,j}(t)\right|^2 = \sum_{n,l} e^{-it(E_n-E_l)}\langle k|q_n\rangle\langle q_n|j\rangle\langle j|q_l\rangle\langle q_l|k\rangle. \tag{2}$$

The above equations give the general expressions of the classical and quantum transition probabilities, which explicitly depend on the eigenvalues and eigenvectors of the transfer matrix or Hamiltonian. A particular feature related to the transport is the return probability, which is the probability of finding the exciton at the initial node. The transition probability depends on the specific topology of the generated single network, therefore it is appropriate to consider its ensemble averages.

3. Averaged return probabilities

The average of the classical and quantum return probabilities $p_{j,j}(t)$ and $\pi_{j,j}(t)$ over all nodes of the network are

$$\bar{p}(t) = \frac{1}{N}\sum_n e^{-tE_n}\sum_j \langle q_n|j\rangle\langle j|q_n\rangle = \frac{1}{N}\sum_n e^{-tE_n}, \tag{3}$$

and

$$\bar{\pi}(t) = \frac{1}{N}\sum_j \pi_{j,j}(t) = \frac{1}{N}\sum_j \left|\alpha_{j,j}(t)\right|^2 = \frac{1}{N}\sum_{n,l} e^{-it(E_n-E_l)}\sum_j \langle j|q_n\rangle\langle q_n|j\rangle\langle j|q_l\rangle\langle q_l|j\rangle. \tag{4}$$

The classical $\bar{p}(t)$ is only dependent on the eigenvalues and decays monotonically from $\bar{p}(0) = 1$ to the equipartition $\lim_{t\to\infty}\bar{p}(t) = 1/N$. The quantum $\bar{\pi}(t)$ is dependent on the eigenvalues and eigenvectors, which is cumbersome in the numerical calculations. The above equations present the average of return probabilities over all nodes on a specific single network. In order to reduce the statistical fluctuation, we further average the return probabilities over distinct single networks, i.e.,

$$\langle\bar{p}(t)\rangle = \frac{1}{R}\sum_{r=1}^{R}\bar{p}^r(t), \tag{5}$$

and

$$\langle\bar{\pi}(t)\rangle = \frac{1}{R}\sum_{r=1}^{R}\bar{\pi}^r(t), \tag{6}$$

where the index r denotes the rth generated ER network. Throughout this Letter, we denote the average over network nodes by a bar (e.g., $\bar{k}$, $\bar{p}(t)$, $\bar{\pi}(t)$, etc.), and the average over different realizations by a bracket (e.g., $\langle\bar{p}(t)\rangle$) while the actual values by undecorated characters.

Fig. 1(a) shows the ensemble averaged return probabilities $\langle\bar{p}(t)\rangle$ and $\langle\bar{\pi}(t)\rangle$ on ER networks of size $N = 100$ with average degree $\bar{k} = 10$, 20 and 30. For classical transport $\langle\bar{p}(t)\rangle$ reaches the equipartition $\lim_{t\to\infty}\bar{p}(t) = 1/N$ very quickly. The curves at intermediate times follow stretched exponential decay, which differs from power law decay ($t^{-0.5}$) for the cycle graph [26]. The exponential decay of $\langle\bar{p}(t)\rangle$ indicates that a classical excitation will quickly spread the whole network and occupy each node with an uniform probability $1/N$ in a short time. It is evident that the excitation reaches the equipartition $1/N$ more quickly on networks with more connections (compare the curves in Fig. 1(a)). For quantum transport $\langle\bar{\pi}(t)\rangle$ also decays quickly in the intermediate times and then reach a final plateau. This plateau is larger than the equipartitioned probability $1/N$. After a careful examination, we find such plateau corresponds to a constant value $\langle\bar{\pi}(t)\rangle \approx 0.065 \pm 0.01$. Increasing the average degree $\bar{k}$ nearly does not change this value (compare the curves in Fig. 1(a)). We note that here $\langle\bar{\pi}(t)\rangle$ is smooth and does not display the oscillatory behavior, in contrast to the case for the cycle graph in which the