Quantum and classical diffusion on small-world networks

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We study numerically quantum diffusion of a particle on small-world networks by integrating the timedependent Schrödinger equation with a localized initial state. The participation ratio, which corresponds to the number of visited sites in the case of classical diffusion, as a function of time is measured and the corresponding diffusion time, τ is computed. In a local regular network, i.e., in the network with the rewiring probability p=0, the diffusion time depends on the network size N as $\tau \sim N$, while the behavior $\tau \sim \log N$ is observed as p becomes finite. Such fast diffusion of a particle on a complex network suggests that the small-world transition is also the fast-world transition from a dynamic point of view. The classical diffusion behavior is also studied and compared with the quantum behavior.

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There has been a surge of research activity on various aspects of complex networks since some important features of real networks were successfully explained by simple model networks.^{1–3} In particular, the Watts-Strogatz (WS) model² was the first to produce networks with small-world behavior, characterized by the path length increasing logarithmically with the network size. Subsequently, a number of studies have been performed on such complex networks, focused mostly on structural properties of the networks. On the other hand, vertices of a real network may have some internal degrees of freedom, interwoven with the structure of the network. Motivated by this observation, a group of researchers has also investigated statistical mechanical models defined on complex networks. For example, spin models such as the Ising model and the XY model on WS networks have been shown to undergo finite-temperature phase transitions of the mean-field nature,^{4,5} disclosing the role of long-range interactions along the shortcuts. In some cases the time development of the network structure may be coupled to the dynamics of degrees of freedom defined on vertices. Still the study of vertex dynamics without considering its influence on the network structure can be useful as a first step toward complete understanding. In this spirit, dynamic models defined on networks draw much attention: Epidemic spreading as well as classical diffusion on complex networks have been studied,^{6,7} and very recently, the dynamic universality class of the XY model on the WS network has been identified.⁸

Properties of a quantum-mechanical model put on a complex network have also been studied with respect to the spectral properties of the Laplacian operator⁹ and the localization-delocalization transition in the presence of site disorder.¹⁰ In this work we consider quantum as well as classical diffusion of a particle on the WS network without site disorder, and investigate how the diffusion time scales with the network size. It is well known that as soon as the WS network (of size *N*) has a finite fraction of shortcuts, it undergoes the small-world transition in which the characteristic path length *l* changes its behavior from $l \sim N$ to $\log N$.^{2,11} From the dynamic point of view, this change from largeworld to small-world behavior is expected to be accompanied by a sharp change in the behavior of the diffusion time: If the world is small, the traveling time around the world should also be short. Indeed the diffusion time τ associated with the participation ratio is observed to change the size dependence from $\tau \sim N$ to log N, which is to be compared with the case of classical diffusion: $\tau \sim N^2$ to N.

The low-dimensional tight-binding electron system has been studied extensively in relation to the localization transition in the presence of disorder. In the absence of disorder, the energy eigenstate of a tight-binding electron on a local regular lattice is always in the extended state due to the Bloch theorem. Here we consider the tight-binding electron on the WS network, described by the time-dependent Schrödinger equation

$$i\frac{\partial|\Psi\rangle}{\partial t} = H|\Psi\rangle,\tag{1}$$

where we have set $\hbar \equiv 1$ and the ket $|\Psi\rangle$ has the position representation $\Psi_n \equiv \langle n | \Psi \rangle$ at the *n*th vertex. The Hamiltonian in the position representation takes the form

$$H_{nn'} = H_{n'n} = \begin{cases} \Delta & \text{for } n' \in \Lambda_n, \\ 0 & \text{otherwise,} \end{cases}$$
(2)

where the on-site energy has been assumed to be uniform and set equal to zero $(H_{nn} \equiv 0)$, Δ is the hopping energy, and Λ_n represents the set of neighbors of vertex *n*. For example, in a local regular network with the connection range r=1, we have $\Lambda_n = \{n-1, n+1\}$.

The WS network is constructed according to the standard procedure in Ref. 2: A one-dimensional (1D) local regular network with the connection range r is built first, then with the rewiring probability p each local edge is rewired to another randomly chosen vertex. (See Fig. 1, illustrating the case r=2.) Once the WS network is constructed in this way, we normalize the time t in units of $1/\Delta$, and integrate the time-dependent Schrödinger equation given by Eqs. (1) and (2) numerically by means of the fourth-order Runge-Kutta method with the discrete time step $\delta t=0.01$, starting from



FIG. 1. Construction of the Watts-Strogatz (WS) network. Starting from the regular one-dimensional lattice in (a) with the connection range r=2, we visit each edge and rewire it with given probability p, thus generating shortcuts in (b). Via this procedure a complicated network structure emerges, as shown in (c).

the initial condition that the electron is localized at a randomly chosen vertex *m*, i.e., $\Psi_n(t=0) = \delta_{n,m}$. For simplicity, we set the initial position $m \equiv 0$.

In the absence of shortcuts, the analytic solution of Eq. (1) is easily found:¹² In the simplest case of r=1, the Fourier transformation $\tilde{\Psi}_k = \sum_n \Psi_n e^{ink}$ yields

$$i\frac{\partial\tilde{\Psi}_{k}}{\partial t} = (e^{ik} + e^{-ik})\tilde{\Psi}_{k} = 2\cos k\tilde{\Psi}_{k}, \qquad (3)$$

which in turn leads to

$$\tilde{\Psi}_k(t) = \tilde{\Psi}_k(0) e^{-2it\cos k}.$$
(4)

The inverse Fourier transformation

$$\Psi_n = \frac{1}{N} \sum_k \tilde{\Psi}_k e^{-ink} \tag{5}$$

in the limit of $N \rightarrow \infty$, combined with the Jacobi-Anger expansion $e^{iz \cos \theta} = \sum_{m=-N}^{N} i^m J_m(z) e^{im\theta}$ gives the solution

$$\left|\Psi_{n}(t)\right| = \left|J_{n}(2t)\right| \tag{6}$$

with the Bessel function J_n of the order *n*. For r=2, it is straightforward to obtain $\Psi_n(t) = \sum_p (-i)^{n-p} J_{n-2p}(2t) J_p(2t)$.

As time proceeds, the initial localized state diffuses and eventually evolves to an extended state in which $\Psi_n \neq 0$ at any *n*. Figure 2 shows such diffusion of the wave packet on the WS network with the connection range r=2 for the rewiring probabilities p=0 and 0.2. It is clearly shown that diffusion occurs much faster in Fig. 2(b), namely, for $p \neq 0$. In this case as soon as the wave packet diffuses to a nearby end point of a shortcut, the other end of the shortcut becomes a new center for diffusion at the next time step, resulting in a faster spread of the wave packet.

To describe the diffusion of the wave packet, one may measure the variance of the wave packet, ¹³ $\sigma^2(t) = \langle \Psi(t) | x^2 | \Psi(t) \rangle - \langle \Psi(t) | x | \Psi(t) \rangle^2$ with the onedimensional position x on the network. However, the variance σ^2 tends to overestimate the diffusion of the wave packet. As an example, consider a state in which the wave packet is localized at two vertices separated by a distance O(N). Although the state is well localized in the sense that the particle can be detected only at a few sites, the variance has a very large value $O(N^2)$. This is in contrast with a local network, where the particle can hop to only locally con-



FIG. 2. Spread of the wave packet initially localized at x=0 on the Watts-Strogatz network with the connection range r=2 for the rewiring probability p = (a) 0 and (b) 0.2. In both (a) and (b), the three curves describe the wave packet at times t=1.0, 5.0, and 10.0, respectively (from top to bottom). It is observed that the wave packet diffuses much faster in (b) than in (a). For clarity, $2|\Psi|^2$ (instead of $|\Psi|^2$ for t=1.0) is plotted for t=5.0 and 10.0.

nected nearby sites and thus σ^2 may be used as a measure of the diffusion without any confusion. To avoid this difficulty with σ^2 , we instead consider the participation ratio $P_Q(t)$ as a function of time:

$$P_{Q}(t) \equiv \frac{\sum_{n} |\Psi_{n}(t)|^{2}}{\sum_{n} |\Psi_{n}(t)|^{4}},$$
(7)

which has the value unity for a wave packet localized completely at one site. For a completely extended state, on the other hand, we have $|\Psi_n|^2 \sim 1/N$ and accordingly, the participation ratio $P_Q \sim N$. The initial localized state with $P_Q(t=0)=1$ thus evolves to the extended state with $P_Q(t\to\infty)$ = O(N) as the time-dependent Schrödinger equation is integrated in time.

With Eq. (6) and the asymptotic form of the Bessel function, a lengthy but straightforward calculation leads to the asymptotic behavior $P_Q(t) \sim t$ on the 1D regular network (without shortcuts) regardless of the range. On a *d*-dimensional (regular) network, Eq. (2) still allows the analytic solution $|\Psi_{n_1n_2\cdots n_d}(t)| = |J_{n_1}(2t)\cdots J_{n_d}(2t)|$, producing the behavior $P_Q(t) \sim t^d$. To characterize diffusion, we define the diffusion time τ associated with the participation ratio by the condition

$$P_O(t=\tau) = cN \tag{8}$$

with a constant c between zero and unity. For a d-dimensional network, we thus have the scaling behavior

$$\tau \sim N^{1/d}.$$
 (9)

For the WS network with shortcuts, the participation ratio in Eq. (7) is computed numerically at given time t and the diffusion time τ is measured from the condition in Eq. (8),



FIG. 3. Diffusion time τ versus the network size *N* in the log-log scale. The case p=0, corresponding to the local regular network, exhibits power-law behavior $\tau \sim N$, whereas downward curvatures are present at nonzero values of *p*. Inset: τ versus *N* for p=0.5 in the semilog plot: The behavior $\tau \sim \log N$ is manifested. Error bars are not larger than the symbols.

where we choose the numerical factor c = 0.25. Another choice for the value of c does not make any qualitative difference in the scaling behavior of τ , only if it is not too close to zero or unity.

In Fig. 3, we display the diffusion time τ depending on the size N at various values of the rewiring probability p. Here the participation ratio $P_{Q}(t)$ has been computed for 3000 different network realizations with given parameters N, r, and p, over which averages have been taken. It is observed that the dependence on N changes crucially as p is increased: At p=0, the linear behavior $\tau \sim N$ is indeed observed in agreement with the analytical result while the inset manifests the dependence $\tau \sim \log N$ for p = 0.5. We have not systematically investigated the scaling behavior at smaller values of *p*; this is difficult from the computational point of view since Nneeds to be greatly increased to avoid finite-size effects. Nevertheless it is very plausible to conclude that the behavior $\tau \sim \log N$ persists as far as p is nonzero. The observed change of the scaling behavior from $\tau \sim N$ to $\log N$ is very interesting in comparison with the change of the characteristic path length from $l \sim N$ to $\log N$ already observed.² This suggests that the small-world transition at p=0, separating the large-world behavior $(l \sim N)$ from the small-world behavior $(l \sim \log N)$, is also the fast-world transition between the slow-world behavior ($\tau \sim N$) and the fast-world behavior $(\tau \sim \log N)$ from the dynamical point of view. Note also that, in view of Eq. (9) for a d-dimensional system, such logarithmic behavior apparently indicates that the effective dimension of the WS network is infinite, which is consistent with the observation of the mean-field nature.^{4,5}

In Fig. 4, the diffusion time τ versus the rewiring probability p is displayed for various network sizes. As the size N becomes larger, the region described well by the relation $\tau \sim p^{-1}$ covers a broader range of p, suggesting that the power-law behavior $\tau \sim p^{-1}$ is valid at any nonzero value of p in the thermodynamic limit. The monotonic decrease of τ



FIG. 4. Diffusion time τ versus the rewiring probability p in the WS network of various sizes. The behavior $\tau \sim p^{-1}$ is observed in a range of p near p = 1, which expands as the size N is increased.

with p is easily understood: The more shortcut end points, the faster the diffusion, as discussed above. Such anomalous quantum diffusion, observed in this work for complex networks, has also been investigated in various quasiperiodic quantum systems^{13,14} as well as in quantum systems which have classically chaotic counterparts.¹⁵

For comparison, we also briefly consider diffusion of a classical particle on the WS network. The particle is put on a randomly chosen vertex of the WS network constructed as before, then allowed to hop to one of its neighboring vertices, chosen randomly each time. While the return probability in such classical diffusion was examined,⁶ it is appropriate here to consider, by analogy with the quantum-mechanical participation ratio $P_Q(t)$, the number of vertices visited by the particle during time t, denoted by $P_C(t)$. Note that this has two limiting values $P_C(t=0)=1$ and $P_C(t\to\infty)=N$, which are the same as those of P_Q . We thus call P_C the classical participation ratio for convenience. The diffusion time τ for the classical diffusion is then determined by



FIG. 5. Diffusion time τ versus the network size N for classical diffusion. At p=0 the behavior $\tau \sim N^2$ is observed, whereas all curves at $p \neq 0$ show the scaling behavior $\tau \sim N$ for sufficiently large N.



FIG. 6. Classical diffusion time τ versus the rewiring probability *p* for various network sizes. Unlike quantum diffusion, classical diffusion is not well described by the behavior of the diffusion time $\tau \sim p^{-1}$.

$$P_C(t=\tau) = 0.1N,$$
 (10)

where the use of numerical values other than 0.1 again does not change the scaling behavior of τ . In the absence of shortcuts (p=0), the WS network reduces to the simple onedimensional local regular network, where it is known¹⁶ that $P_C(t) \sim t^{1/2}$, and consequently we have the behavior $\tau \sim N^2$.

Figure 5 shows the diffusion time τ versus the size N of the WS network for various values of the rewiring probability p. As in the quantum case, $P_C(t)$ has been computed for 3000 different network realizations and averages over them have been taken. As expected, for p=0 corresponding to the local one-dimensional lattice, the standard behavior $\tau \sim N^2$ is observed. In sharp contrast, at any nonzero value of p the diffusion time displays the behavior $\tau \sim N$, demonstrating that classical diffusion on the WS network changes dramatically as soon as p takes a nonzero value. This behavior τ $\sim N$ is also consistent with the infinite effective dimension of the WS network, in view of the known result that $P_C(t) \sim t$

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TABLE I. Quantum and classical diffusion: The diffusion time τ versus the network size *N*. For comparison, the scaling behavior of the characteristic path length *l* is also presented.

	p = 0	$p \neq 0$
Quantum	$ au{\sim}N$	$\tau \sim \log N$
Classical	$ au \sim N^2$	$ au \sim N$
Characteristic path length	$l \sim N$	$l \sim \log N$

for dimensions $d \ge 3$.¹⁶ Comparing this observation for classical diffusion with the previous one for quantum diffusion, one can in both cases draw the conclusion that the smallworld transition at p=0, associated with the change of the scaling behavior of the characteristic path length l, is accompanied by the fast-world transition in the dynamic view point, where the exponent a in the relaxation behavior $\tau \sim N^a$ changes to a-1. On the other hand, Fig. 6, where τ versus p for classical diffusion is plotted, shows that the behavior $\tau \sim p^{-1}$ observed for quantum diffusion (see Fig. 4) does not appear in classical diffusion.

In summary, we have investigated both quantum diffusion and classical diffusion on Watts-Strogatz small-world networks. To describe these, we have introduced the participation ratio and determined the diffusion time. The obtained scaling behaviors of the diffusion time, as summarized in Table I, show dramatic changes as one increases the rewiring probability from zero to a nonzero value. This is reminiscent of the small-world transition in the scaling behavior of the characteristic path length l from the small-world regime l $\sim N$ to the large-world regime $l \sim \log N$, and suggests that the small-world transition can also be termed the fast-world transition.

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