Time Reversibility of Quantum Diffusion in Small-world Networks

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Time-irreversible phenomena in nature, such as spread of an ink blob in water and aging of living organisms, are ubiquitous in our macroscopic world [1]. We always see the ink blob spread in a tea cup and people get older, not the other way around. These time-irreversible behaviors look puzzling because all these dynamics are based on microscopic equations of motion, quantum or classical, that contain time-reversal symmetry. In the late 19th century, this seemingly paradoxical observation of time-reversal thermodynamics perplexed many scientists until a breakthrough was made by Boltzmann. It is now well-known that the directionality of the arrow of time in the second law of thermodynamics can be understood by the huge difference in the numbers of allowed microscopic states between the initial and the final macroscopic states.

Recently, the quantum and classical time-reversal dynamics of a diffusion system and a spin system have been studied to answer the long-standing question of where does the irreversibility come from [2–5]. In Ref. 3, quantum diffusion systems were shown to display the universal behavior of time irreversibility in terms of perturbation strength. Because the complex networks have drawn much interest, there have been studies of quantum systems in Watts-Strogatz (WS) small-world networks [6]. Localization phenomena of quantum systems in small-world networks have been studied [7, 8], and quantum diffusion problems have been investigated in various ways in WS networks [9–12].

In the present work, we aim to study the time-reversibility of the quantum diffusion problem in WS networks. The diffusion of a wave packet has been shown to occur much faster in WS networks than in a regular network [10, 11]: A suitably defined diffusion time in a quantum system shows \( \tau \sim \log N \) in the former while \( \tau \sim N \) for the latter structure. An abrupt change in the scaling behavior of \( \tau \) has been shown to occur as soon as the rewiring probability becomes nonzero. In other words, a transition from the slow world \( (\tau \sim N) \) to the fast world \( (\tau \sim \log N) \) occurs at null rewiring probability simultaneously with a structural transition from the large world \( (l \sim N) \) to the small world \( (l \sim \log N) \), with \( l \) being the average path length connecting two arbitrarily chosen vertices. Consequently, a change in the scaling behavior of \( \tau \) reflects a dynamical aspect of the small-world transition in WS networks. In this work, we examine the effect of shortcuts on the time reversal dynamics of the tight-binding electron at different perturbation strengths.

The time evolution of the tight-binding electron in a network structure is governed by the following time-dependent Schrödinger equation:

\[
\frac{i\hbar}{\mathbf{\partial}} \frac{\partial \Psi}{\partial t} = H \Psi, \tag{1}
\]

where \( \hbar \) is the Planck constant, and the quantum mechanical ket \( \Psi \) and the Hamiltonian \( H \) in position representation are written as \( \Psi_n \equiv \langle n|\Psi \rangle \) and

\[
H_{nn'} = H_{n'n} = \begin{cases} 
\Delta & \text{for } n' \in \Lambda_n \\
0 & \text{otherwise,}
\end{cases}
\tag{2}
\]

respectively. Here, \( n \) is the vertex index, \( \Lambda_n \) is the set of directly connected vertices of \( n \), and the on-site energy has been assumed to be uniform and set equal to zero. As a further simplification, we also assume that the hopping energy \( \Delta \) does not depend on \( n \) or \( n' \). Henceforth, we use the dimensionless units: the time is measured in units of \( \hbar/\Delta \), the position in units of the lattice spacing \( a \) of the one-dimensional (1D) regular lattice without shortcut, and the momentum in units of \( \hbar/a \).

Once the WS network for a given rewiring probability \( p \) is constructed following the standard procedure (see
Ref. [3], we perform the numerical integration of the time-dependent Schrödinger equation starting from the initial localized wave packet at time $t = 0$ ($\Psi_n = \delta_{n,0}$) by using the fourth-order Runge-Kutta algorithm with the discrete time step $dt = 0.01$. Except for $p = 0$, all results are obtained from the average of 1000 different network realizations. We use the time-reversal test similarly to Ref. [2]. At the reversal time $T$, a momentum perturbation of the strength $\eta$ is made by applying the operator $\exp(i\eta \hat{x})$ to $|\Psi(T)\rangle$ with the position operator $\hat{x}$. For convenience, we measure $t$ in the forward direction even after the reversal time $T$ so that at $t = 2T$, the system goes back to the initial state in the absence of the perturbation (i.e., when $\eta = 0$). During the numerical time integration, we compute the participation ratio

$$
\Pi(t) = \frac{\sum_{n=1}^{N} |\Psi_n(t)|^2}{\sum_{n=1}^{N} |\Psi_n(t)|^4},
$$

which has been frequently used in the study of localization phenomena. When the wavefunction is completely localized, $\Pi$ takes the value of unity. On the other hand, as the wavefunction spreads in space and the quantum system becomes extended, $\Pi$ is known to be $O(N)$. The time irreversibility $I$ is then defined as

$$
I \equiv |\Pi(2T) - \Pi(0)|.
$$

It is to be noted that $\Pi(t < T)$ is independent of $\eta$ whereas $\Pi(2T)$ and $I$ are functions of $\eta$. When $\eta = 0$, $I$ takes the value zero, meaning the null irreversibility (or the complete reversibility), because $\Pi(2T) = \Pi(0)$. As $\eta$ is increased from zero, the perturbed momentum at $T$ makes it difficult for the system to go back to the initial quantum state; thus, $I$ is expected to increase.

Figure 1 displays $\Pi(t)$ in Eq. (3) (a) for the local 1D regular network corresponding to the WS network at the rewiring probability $p = 0$ and (b) for the WS network at $p = 0.2$. Although not clearly discernible, each of Fig. 1(a) and (b) has 101 different curves corresponding to $\eta = 0.0, 0.001, 0.002, \ldots, 0.1$ (from bottom to top). We also show the time irreversibility $I$ at various values of $p$ in Fig. 1(c). The system size $N = 1600$ and the reversal time $T = 2$ are used. We first observe that $\Pi(T)$ is about four times larger for $p = 0.2$ than for $p = 0.0$, which is explained by the fast diffusion in the WS network structure, as discussed in Ref. [3]. At both (a) $p = 0$ and (b) $p = 0.2$, time reversal dynamics is shown to give rise to a larger reflection asymmetry of $\Pi(t)$ around $t = T$ as $\eta$ is increased. This is not surprising because a larger momentum perturbation will surely make the time reversed quantum state at $t = 2T$ more different from the initial state at $t = 0$. A more interesting observation one can make from the comparison of Fig. 1(a) and (b) is that the deviation of $\Pi(2T)$ from $\Pi(0)$ is much bigger for the WS network ($p = 0.2$) than for the regular network ($p = 0.0$). This clearly indicates that the structural irregularity in the WS network plays an important role in making the perturbed dynamics deviate severely from the unperturbed one. The enhancement of the irreversibility in the WS network is more clearly seen in Fig. 1(c) for $I$ versus $\eta$ at various rewiring probabilities $p$. Figure 1(c) shows that the irreversibility is a monotonically increasing function of the rewiring probability $p$. In other words, the enhanced structural randomness caused by more shortcuts drives the quantum diffusion dynamics in the WS network to become more sensitive to the momentum perturbation. Interestingly,
the WS network at a sufficiently larger rewiring probability $p$ behaves very differently from the local regular lattice: For $p > 0$, $I$ increases linearly with increasing $\eta$ for the weakly-perturbed region and then soon saturates to a finite value. In contrast, for $p = 0$, $I$ increases linearly with increasing $\eta$ without showing saturation. However, these findings need to be carefully examined in view of the finite scales in the system, i.e., finiteness of the length scale ($N$) and the time scale ($T$).

It should be noted that in WS networks there is an additional length scale other than the microscopic length scale of the lattice spacing $\alpha$ and the macroscopic length scale of the system size $N$. When a nonzero rewiring probability $p$ is given, the number of shortcuts is proportional to $pN$, which determines the third length scale of the average distance $\xi$ between the two endpoints of short-cuts, i.e., $\xi \sim N/pN = 1/p$. If the tail part of the wavefunction of the tight-binding electron does not have enough time to arrive at the closest shortcut endpoint, the system should behave just like a 1D regular lattice. Also, quantum diffusion in a regular 1D system is known to have a diffusion time proportional to the system size to become fully extended ($\tau \sim N$), which indicates that the wavepacket in the 1D system spreads on a distance scale $\ell \sim T$ before reversal time. Accordingly, if $T \sim \ell \lesssim 1/p$, the system behaves just like a 1D regular lattice while it changes its behavior as $T \sim 1/p$ is crossed. Let us consider several cases: (i) For $pT \lesssim 1$, the system behaves like a 1D system because $T$ is short enough that the wavepacket does not have time to arrive at a shortcut endpoint. Furthermore, in this case of short-time diffusion, all observed results should be independent of $N$ as long as $T \ll N$; i.e., $T$ is too short for the particle to feel the finiteness of the system. (ii) For $pT \gtrsim 1$, the tight-binding particle now begins to meet shortcut endpoints and the diffusion behavior changes. As soon as the WS network begins to have a finite fraction of short-cuts, the quantum diffusion behavior is known to rapidly change so that the diffusion time $\tau$ increases only logarithmically with increasing $N$. This implies that the wavefunction spreads in a distance that increases exponentially with time. We, thus, conclude that this very fast diffusion occurs when $pT \gtrsim 1$ and that the particle can arrive at the other side of the system, giving rise to an $N$-dependence in the irreversibility. Consequently, the size-independence of $I$ in the region of $pT \lesssim 1$ is changed as we enter the intermediate region of $pT \gtrsim 1$. (iii) For the limiting case of $pT \gg 1$, the wavefunction of the particle has already completely spread; thus, the irreversibility should not depend on $pT$. In this long-time limit, the wavefunction becomes fully extended, and the participation ratio is $\Pi \sim N$. Consequently, for a big enough system, $I(pT)/N$ saturates as $pT$ becomes larger, approaching a value that does not depend on $N$.

The results for the irreversibility $I$ versus $pT$ curve at $\eta = 0.1$ shown in Fig. 2 clearly fit the above hand-waving scaling arguments well. In Figs. 2(a) and (b), $I$ is shown to be independent of $N$ for $pT \lesssim 1$ whereas we see a clear size dependence for $pT \gtrsim 1$. As $pT$ is increased even further, $I$ saturates to some values that depend on $N$, as clearly seen in Fig. 2(b). Figure 2(c) shows that the saturated value of $I/N$ in the limit of $pT \gg 1$ is independent of $N$.

In summary, we studied the time reversal dynamics of the tight-binding electron system in the WS small-world networks. Initially, the localized quantum mechanical state of the electron evolves in time until the momentum perturbation of the strength $\eta$ is made at $T$, at which time reversal operation is also made. The 1D regular lattice and the WS small-world network exhibit different behaviors: the irreversibility, measured by the difference between the participation ratio of the final and the initial states, is found to be bigger in the latter network due to
the structural randomness caused by the random short-
cuts. It is also found and argued that the irreversibility
does not depend on the system size for $pT \lesssim 1$ and that
it saturates to a value as $pT$ becomes larger.

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[1] J. L. Lebowitz, Physica A. 263, 516 (1999).
[2] C. Petitjean and Ph. Jacquod, Phys. Rev. Lett. 97, 124103 (2006).
[3] H. S. Yamada and K. S. Ikeda, Phys. Rev. E 82, 060102(R) (2010).
[4] M. Hiller, T. Kottos, D. Cohen, and T. Geisel, Phys. Rev. Lett. 92, 010402 (2004).
[5] G. Waldherr and G. Mahler, EPL 89, 40012 (2010).
[6] D. J. Watts and S. H. Strogatz, Nature (London) 393, 440 (1998).
[7] O. Giraud, B. Georgeot, and D. L. Shepelyansky, Phys Rev. E 72, 036203 (2005).
[8] C-P. Zhu and S-J. Xiong, Phys. Rev. B 63, 193405 (2001).
[9] R. Monasson, Eur. Phys. J. B 12, 555 (1999).
[10] B. J. Kim, H. Hong, and M. Y. Choi, Phys. Rev. B 68, 014304 (2003).
[11] O. Mülken and A. Blumen, Phys Rev. E 73, 066117 (2006).
[12] O. Mülken, V. Pernice, and A. Blumen, Phys Rev. E 76, 051125 (2007).