Continuous-time quantum walks on a cycle graph

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(Received 9 June 2005; revised manuscript received 1 November 2005; published 11 January 2006)

We present an analytical treatment of quantum walks on a cycle graph. The investigation is based on a realistic physical model of the graph in which decoherence is induced by continuous monitoring of each graph vertex with a nearby quantum point contact. We derive an analytical expression of the probability distribution along the cycle. An upper-bound estimate to the mixing time is shown.

DOI: 10.1103/PhysRevA.73.012313 PACS number(s): 03.67.Lx, 05.40.Fb, 03.65.Xp, 05.45.Mt

Quantum walks have been widely discussed recently as a promising technique for development of quantum algorithms [1,2]. Both discrete-time quantum coined walks and continuous-time quantum walks have been argued to give an algorithmic speedup with respect to their classical counterparts [3]. Unlike common discrete-time quantum algorithms [4] that are very sensitive to environmental quantum noise [5], quantum walks show some promise in dealing with decoherence processes. Numerical studies of discrete-time quantum walks on a cycle and hypercube have shown that a small amount of decoherence may be useful [6]. In this paper we present a theoretical investigation of continuous-time quantum walks on a uniform cycle graph C_N. We derive the expression for the probability distribution and obtain an upper-bound estimate to the mixing time.

In our investigation, the cycle is represented by a ring-shaped array of identical tunnel-coupled quantum dots (QDs); see Fig. 1. The walks are performed by an electron initially placed in one of the dots. Each dot is continuously monitored by an individual point contact (PC), which introduces decoherence to the electron's evolution as discussed in Ref. [7]. The analytical expression for the probability distribution is obtained for a cycle of arbitrary size, i.e., the number of nodes may be large. The latter property allows one to study dynamics and mixing on large graphs, avoiding the usual limitations on size arising in numerical simulations [6].

The QD cycle with "attached" PCs can be, in principle, fabricated with the help of gate-engineering techniques in semiconductor heterostructures [8]. Such techniques allow the formation of QDs and PCs electrostatically by placing metal gates on the structure with a two-dimensional electron gas (2DEG). By changing the potential on the gates one can allocate areas of 2DEG, creating the necessary confinement profile. The simplest example of such a structure containing two QDs was investigated experimentally in Ref. [9]. Our key assumptions are as follows: identical PCs are formed far enough from the QD structure so that the tunneling between them is negligible; Coulomb interaction between electrons in the QD and PC is taken into account.

We begin with formulating the basic equations of our model. The Hamiltonian of an electron placed in the QD cycle is

$$H_{cycle} = \frac{1}{4}\sum_{j=0}^{N-1} (c_{j+1}^{\dagger} c_j + c_j^{\dagger} c_{j+1}), \tag{1}$$

where $c_j^{\dagger}$ (c_j) are creation (annihilation) operators for an electron on site j, N is the number of QDs in the cycle, and $c_N \equiv c_0$. We renormalize the time for convenience, so that it becomes dimensionless, and all the amplitudes further on are given in terms of the hopping amplitude between neighboring QDs.

The point contact, placed next to each QD, consists of two reservoirs of electrons, source and drain, that are coupled through the potential barrier shaped by PC gates (see Fig. 1). The Hamiltonian of the jth PC can be written as

$$H_{PC,j} = \sum_l E_{l,j} a_{l,j}^{\dagger} a_{l,j} + \sum_r E_{r,j} a_{r,j}^{\dagger} a_{r,j} + \sum_{lr} \Omega_{lr,j} (a_{l,j}^{\dagger} a_{r,j} + a_{r,j}^{\dagger} a_{l,j}), \tag{2}$$

where $a_{l,j}^{\dagger}$ $(a_{l,j})$ and $a_{r,j}^{\dagger}$ $(a_{r,j})$ are creation (annihilation) operators in the left (source) and right (drain) reservoirs of the jth PC. $\Omega_{lr,j}$ are the tunneling amplitudes between states l and r of the jth PC. In our discussion we consider all elec-

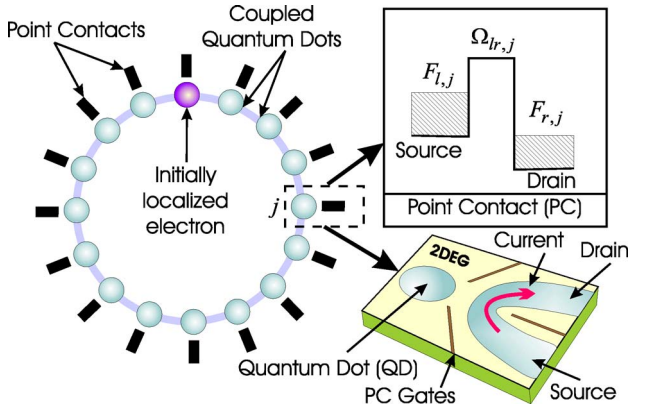

FIG. 1. (Color online) Continuous-time quantum walk architecture: ring of quantum dots, each of which is monitored by the corresponding point contact that introduces decoherence. $F_{l,j}$ and $F_{r,j}$ are chemical potentials of the source and drain of the jth point contact. The presence of an electron in the jth quantum dot affects the source-to-drain tunneling amplitude $\Omega_{lr,j} \rightarrow \Omega_{lr,j} + \delta\Omega_{lr,j}$ of the jth point contact.

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trons to be spinless fermions. Source and drain reservoirs are kept at zero temperature with chemical potentials $F_{l,j}$ and $F_{r,j}$. By allowing weak Coulomb interaction between electrons in the PC and QD we observe the presence of the electron in the jth QD as it changes the tunneling amplitude through the barrier of the adjoining PC, i.e., effectively $\Omega_{lr,j} \to \Omega_{lr,j} + \delta\Omega_{lr,j}$, so that $\delta\Omega_{lr,j}$ represents the rise of the potential barrier in the PC when the corresponding QD is occupied. The correction is assumed to be small compared to the other amplitudes in the problem. This process introduces weak measurement on the electron in each node of the graph, and, therefore, results in some loss of coherence in electron evolution. Summarizing the above discussion, we produce the following correction to the PC Hamiltonian (2):

$$H_{int,j} = \sum_{lr} \delta\Omega_{lr,j} c_j^\dagger c_j (a_{l,j}^\dagger a_{r,j} + a_{r,j}^\dagger a_{l,j}). \tag{3}$$

The total Hamiltonian is

$$H = H_{cycle} + \sum_{j=0}^{N-1} (H_{PC,j} + H_{int,j}). \tag{4}$$

In our investigation we assume that all PCs are identical, and that the hopping amplitudes $\Omega_{lr,j}$ are only weakly dependent on states l,r, which allows us to replace $\Omega_{lr,j}$ and $\delta\Omega_{lr,j}$, as well as $F_{l,j}$ $(F_{r,j})$, by their averages: $\bar{\Omega}$, $\delta\bar{\Omega}$, and $\bar{F}_l$ $(\bar{F}_r)$. Considering the continuous measurement of an electron in a double-well potential by a point contact described above, Gurvitz has shown [7] that for the case of large bias voltages $\bar{F}_l - \bar{F}_r$, the evolution of the reduced density matrix traced over all states of source and drain electrons is given by Bloch-type rate equations. Applied to our model this technique yields the following equation for the reduced density matrix:

$$\frac{d}{dt}\rho_{\alpha\beta} = \frac{i}{4}(\rho_{\alpha\beta+1} - \rho_{\alpha+1\beta} - \rho_{\alpha-1\beta} + \rho_{\alpha\beta-1}) - \Gamma(1-\delta_{\alpha\beta})\rho_{\alpha\beta}, \tag{5}$$

where α,β number the sites on the cycle, running from 0 to $N-1$; $\Gamma = \delta\bar{\Omega}^2(\bar{F}_r - \bar{F}_l)^2 f_S f_D$; and f_S (f_D) stands for the density of states in source (drain) reservoirs. We also set $\hbar = 1$ for convenience.

For further discussion, it is convenient to introduce real variables, defining

$$\rho_{\alpha\beta} \equiv i^{\alpha-\beta} S_{\alpha\beta}. \tag{6}$$

Considering (6) we obtain

$$\frac{dS_{\alpha\beta}}{dt} = \sum_{\mu,\nu=0}^{N-1} (L_{\alpha\beta}^{\mu\nu} + U_{\alpha\beta}^{\mu\nu}) S_{\mu\nu}, \tag{7}$$

where α,β,μ,ν run from 0 to $N-1$, and we have $L_{\alpha\beta}^{\mu\nu}$ and $U_{\alpha\beta}^{\mu\nu}$ defined as

$$L_{\alpha\beta}^{\mu\nu} = \frac{1}{4}(\delta_{\alpha,\mu}\delta_{\beta,\nu-1} + \delta_{\alpha,\mu-1}\delta_{\beta,\nu} - \delta_{\alpha,\mu}\delta_{\beta,\nu+1} - \delta_{\alpha,\mu+1}\delta_{\beta,\nu}), \tag{8}$$

$$U_{\alpha\beta}^{\mu\nu} = -\Gamma\delta_{\alpha,\mu}\delta_{\beta,\nu}(1-\delta_{\alpha,\beta}). \tag{9}$$

As mentioned earlier, we initialize the system by localizing the electron in one of the quantum dots and allow it to evolve, spreading all over the cycle. Therefore, the reduced density matrix elements at $t=0$ are set as follows:

$$\rho_{\alpha\beta}(0) = S_{\alpha\beta}(0) = \delta_{\alpha,0}\delta_{\beta,0}. \tag{10}$$

Condition (10) simply states that the electron is initially localized in dot 0. The choice of the initial condition in the form of Eq. (10) is convenient for further calculations and, in fact, is quite general. Indeed, the symmetry of the system with respect to cyclic rotations allows us to construct the solution to the reduced density matrix for any classical, i.e., with zero off-diagonal elements, initial distribution. The solution for an arbitrary distribution is given by

$$\sum_{j=0}^{N-1} C_j \rho_{\alpha+j\beta+j}(t), \tag{11}$$

where C_j represents the initial probability distribution over the cycle.

Equation (7) can be solved perturbatively in the low-decoherence (quantum) regime, considering $\Gamma N \ll 1$. The zero-order solution is given as an expansion on the eigenvectors of $L_{\alpha\beta}^{\mu\nu}$, defined by

$$\sum_{\mu,\nu=0}^{N-1} L_{\alpha\beta}^{\mu\nu} V_{\mu\nu}^{(mn)} = \lambda_{(mn)}^0 V_{\alpha\beta}^{(mn)}, \tag{12}$$

where $0 \leqslant m,n \leqslant N-1$. From Eq. (12), after some algebra, one can show that the eigenvalues $\lambda_{(mn)}^0$ are

$$\lambda_{(mn)}^0 = i \sin\frac{\pi(m+n)}{N} \cos\frac{\pi(m-n)}{N}, \tag{13}$$

and the eigenvectors $V^{(mn)}$ are given by

$$V_{\mu\nu}^{(mn)} = \frac{1}{N} e^{(2\pi i/N)(m\mu+n\nu)}. \tag{14}$$

Calculation of the corrections requires careful investigation of the unperturbed spectrum (13). The analysis of (13) and (14) allows us to highlight several important subsets of certain degeneracy which lead to nonzero off-diagonal matrix elements of (9) on the basis of (14). First of all, one can notice the symmetry of (13) with respect to index exchange, while the eigenvectors (14) are clearly affected by such an operation. Hence, for $n \neq m$ we deal with at least twofold-degenerate eigenvalues. Another subset reveals itself when we consider the eigenvalues (13) with $m=n=0$ or $m+n=N$. The eigenvalues (13) with these relations for indices are all zero and yet the corresponding eigenvectors are not the same.

First-order corrections to the eigenvalues $\lambda_{(nn)}^0$ of spectrum (13) are given, as one can show, by the diagonal matrix elements of (9) calculated on the eigenvectors (14). They are equal to $-\Gamma(N-1)/N$. The perturbation removes the degeneracy of the first subset introducing $-\Gamma(N-1\pm1)/N$ to each pair of $\lambda_{(mn)}^0$ with $n \neq m$ and $n+m \neq N$. Corrections to

the zero eigenvalues are irrelevant to our calculations due to the fact that the corresponding eigenvectors are anyway excluded from the final expression by the initial condition (10). One can simply analyze the expansion of the right-hand side of (10) in terms of the eigenvectors (14), yielding

$$S_{\alpha\beta}(0) = \frac{\delta_{\alpha,\beta}}{N} + \frac{1}{N^2}\sum_{m,n=0}^{N-1}(1 - \delta_{m+n,0} - \delta_{m+n,N})\exp\left(\frac{2\pi i(m\alpha + n\beta)}{N}\right). \quad (15)$$

The solution to (7) is naturally formed by

$$S_{\alpha\beta}(t) = \sum_{m,n=0}^{N-1} C_{(mn)} e^{\lambda_{(mn)}t} Y_{\alpha\beta}^{(mn)}, \quad (16)$$

where $Y_{\alpha\beta}^{(mn)}$ are some linear combinations of eigenvectors (14) and $\lambda_{(mn)}$ representing the corrected spectrum. The expansion coefficients $C_{(mn)}$ are completely defined by expression (15). Finally, the solution to (7) is

$$S_{\alpha\beta}(t) = \frac{\delta_{\alpha,\beta}}{N} + \sum_{m,n=0}^{N-1}\frac{1 - \delta_{m+n,0} - \delta_{m+n,N}}{N}(\delta_{mn}e^{t\lambda_{(mn)}^0 - \Gamma[(N-1)/N]t} + (1 - \delta_{mn})e^{t\lambda_{(mn)}^0 - \Gamma[(N-2)/N]t})V_{\alpha\beta}^{(mn)}. \quad (17)$$

The probability distribution, which is given by the diagonal elements of the reduced density matrix (17), considering (6), is

$$P_j(t) = \frac{1}{N} + \sum_{m,n=0}^{N-1}\frac{1 - \delta_{m+n,0} - \delta_{m+n,N}}{N^2}(\delta_{mn}e^{-\Gamma[(N-1)/N]t} + (1 - \delta_{mn})e^{-\Gamma[(N-2)/N]t}) \times \exp\left(it\sin\frac{\pi(m+n)}{N}\cos\frac{\pi(m-n)}{N} + \frac{2\pi i}{N}(m+n)j\right). \quad (18)$$

Expression (18) is the final result of our analyses. It gives the probability for an electron, initially placed at node 0, to be found on node j at time t. The probability distribution is shown in Fig. 2. As one can see, weak measurement of the system [shown in Fig. 2(b)] leaves the time evolution of the random walk almost unchanged from that of the coherent walk [shown in Fig. 2(a)]. Figure 2(a) shows the evolution of the walk in the absence of decoherence. Figure 2(b) shows the evolution when the system is exposed to weak measurement (decoherence). In the latter case the coherent oscillation pattern is suppressed by effective averaging that leads to the onset of a uniform distribution.

In quantum walk studies, it is often important to analyze the time it takes for the electron, as a walking particle, to spread along the cycle. This is called the "mixing time" [2,6,10], and for continuous-time quantum walks is used to describe two types of processes. The first one, called "instantaneous mixing," refers to the uniform (or nearly uniform) spread of probability of the walking particle that can happen at some particular moment of evolution [10]. The other, "average mixing," is the decay of the time-averaged deviation of the probability distribution from the uniform case [6]. In the latter case, time averaging is required to settle down the coherent oscillations of probability which, otherwise, would not converge to any static distribution. In our case the averaging arises naturally from the fact that the electron walking on the cycle is continuously monitored by the environment, i.e., the PCs.

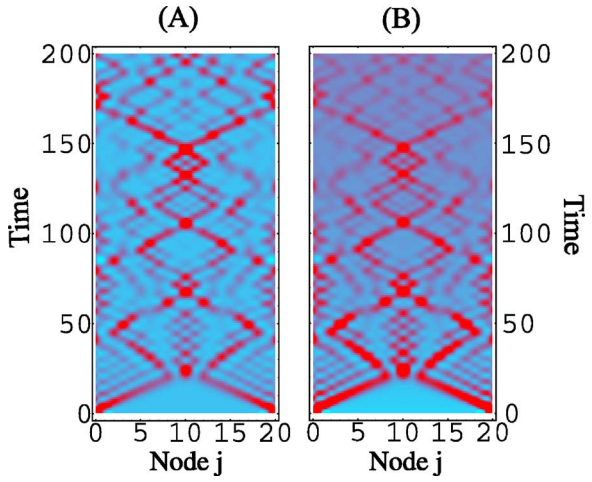

FIG. 2. (Color online) Probability distribution along the cycle as function of time and node number, for $N=20$ and $\Gamma=0$ (a), and 0.01 (b). Here $j \in [0, N-1]$ stands for the node number; darker regions denote higher probabilities. The electron is initially placed at $j=0$. The probability distribution of the walks with some decoherence added, (b), converges to uniform, i.e., to $1/N$.

Let us briefly discuss how fast mixing on a circle can be. One of the apparently necessary (but not at all sufficient) conditions for the walking particle is to have some nonzero amplitude on each node. Therefore, the wave of probability of the particle localized initially in one of the nodes has to travel all over the cycle at least once. We should note that for our range of parameters this has already happened by times of order $1/\Gamma$.

Below, we obtain an upper-bound estimate based on the solution (18). The mixing time t_{mix} is defined [6] as the minimum time that satisfies the mixing condition

$$\sum_{j=0}^{N-1}\left|P_j(t_m) - \frac{1}{N}\right| \leqslant \varepsilon, \quad (19)$$

where ε is some small dimensionless constant that presets the desired degree of mixing, and $1/N$ stands for the uniform distribution. To find the upper-bound estimate, let us analyze the left part of inequality (19). After some algebra with expression (18) one can obtain

$$\left|P_j(t_m) - \frac{1}{N}\right| = e^{-\Gamma[(N-2)/N]t_m}\left|S^2(j,t_m/2) - \frac{2}{N} + \frac{e^{-\Gamma t_m/N} - 1}{N}\left(S(2j,t_m) - \frac{2 - N \bmod 2}{N}\right)\right|, \quad (20)$$

where

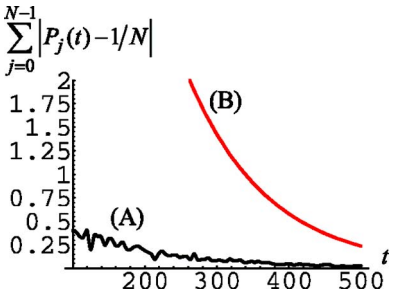

FIG. 3. (Color online) The sum of the absolute deviations of probability from the uniform distribution curve A, with majorizing curve B are shown. Analysis of the latter allows an analytical expression for the upper-bound estimate to the mixing time, which is found to be linear in N. Parameters used are $N=20$ and $\Gamma=0.01$.

$$S(j,t)=\frac{1}{N}\sum_{n=0}^{N-1} e^{it\,\sin(2\pi n/N)+i(2\pi n/N)j}. \tag{21}$$

The absolute value of the sum (21) is always smaller than or equal to unity, which allows us to majorize (20) as follows:

$$\left|P_j(t_m)-\frac{1}{N}\right| \leqslant e^{-\Gamma[(N-2)/N]t_m}\left[1+\frac{2}{N}+\frac{1-e^{-\Gamma t_m/N}}{N}\left(1+\frac{2}{N}\right)\right]. \tag{22}$$

In Fig. 3 we plot the sum of the absolute deviation of the probability distribution from the uniform one, curve A, along with the majorizing expression, curve B. Substituting (22) into (19) we obtain the relation

$$N+2+\frac{N+2}{N}[1-\exp(-\Gamma t_m/N)] \leqslant \varepsilon[\exp(\Gamma t_m/N)]^{N-2}, \tag{23}$$

which always has a solution at some large t_m. The upper bound for the mixing time can be defined as $t_{mix} \leqslant \min t_m$. The latter minimum is estimated considering the fact that the last term of the left-hand side in (23) does not exceed $(N+2)/N$. As a result, assuming $N>2$ we obtain

$$t_{mix} < \frac{3}{\Gamma}\ln\left(\frac{N+4}{\varepsilon}\right). \tag{24}$$

As mentioned above, expression (24) is based on the solution (18). At the same time one can estimate the effect of higher-order corrections. The right-hand side of Eq. (24) yields $3\ln\{(N+4)[1+O(\Gamma)]/\varepsilon\}/\Gamma[1+O(\Gamma)]$. As we see, in low-decoherence mode the mixing time may not exceed a quantity logarithmic in N for a given Γ. This result needs to be explained. Indeed, one would expect the mixing time to develop at least linearly in the size of the cycle. There is no contradiction, however, as long as one notices that the solution is obtained for small Γ, namely, $\Gamma N \ll 1$. Note that by the time Γ^{-1} our walking particle has already reached the opposite site on the cycle (see, for example, Fig. 2). Therefore expression (24) bounds the mixing time as a function of N when Eq. (18) is valid. On the other hand, for a fixed size of the cycle the mixing time is expected to decrease as $1/\Gamma$. Eventually, as Γ increases one goes to the regime of strong measurement with emerging Zeno effect, where the electron is localized by the measurement itself, which obviously destroys mixing. Observing (24), one may speculate that there must be some optimal value for the decoherence parameter Γ which corresponds to the minimum mixing time for a given size of a cycle. This behavior requires careful investigation and goes beyond the scope of the present paper. We should also note that instantaneous mixing (if it exists) can actually happen much earlier as compared to (24). The mixing time in the latter case is determined, primarily, by the pattern of coherent oscillations.

In conclusion, we have studied quantum walks on a cycle graph, represented by a ring-shape array of quantum dots continuously monitored by individual point contacts, which introduce decoherence. An analytical expression for the probability distribution along the cycle has been obtained for a small amount of decoherence. We have shown that at fixed low decoherence rates the upper-bound estimate for the mixing time has a log-linear dependence on the size of the cycle, while on fixing the size, one observes an inverse linear dependence on the decoherence rate.

We are grateful to Christino Tamon for helpful discussions. This research was supported by the National Science Foundation, Grant No. DMR-0121146.

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