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SIMULATING DIFFUSION WITH QUANTUM WALKS ON GRAPHS

YAN WANG
Woodruff School of Mechanical Engineering
Georgia Institute of Technology, Atlanta, GA 30332, USA
Email: yan.wang@me.gatech.edu

The path integral method has been an effective approach to solve the Fokker-Planck equation that simulates the evolution of probability distributions in diffusion processes. Yet the major challenges include the memory requirement to store the transition matrix in a fine-grained state space and a small time step required for the accurate estimation of short-time transition probabilities. Previously, one-dimensional continuous-time quantum walk has been used in diffusion simulation. By combining quantum diffusion and random diffusion, the new simulation approach can achieve acceleration by increasing the time step size significantly. It has been demonstrated that dozens or even hundreds of times longer step sizes can be used. In this paper, a new generic quantum operator is proposed to simulate drift-diffusion processes in high-dimensional space, which combines quantum walks on graphs with traditional path integral approaches. Probability amplitudes in quantum walks can be computed efficiently by spectral analysis. The efficiency of the new simulation method is demonstrated with stochastic resonance problems.

Keywords: Fokker-Planck equation, path integral, quantum walks, stochastic resonance

1 Introduction

Stochastic diffusion processes are universal and appear in various physical, chemical, biological and economical systems. In engineering applications, we usually need to simulate and design system dynamics, such as in modeling suspension of vehicles on rough pavement, analyzing vibration of structures under stochastic load, and designing rotational machinery with random excitation.

Stochastic differential equation (SDE) and Fokker-Planck equation (FPE) are two general approaches to describe the drift-diffusion processes in a stochastic system. SDEs model the system under uncertainty with samples of individual trajectories as a result of the Wiener process, whereas FPEs capture the time evolution of probability distributions directly. Solving SDEs relies on the Monte Carlo sampling of system trajectories. A large number of samples need to be generated to draw statistical conclusions. In contrast, a FPE captures the dynamics of the probability density for all possible states and models the evolution process of the overall distribution.

The main research challenge of solving SDEs and FPEs is to develop efficient and robust numerical methods to obtain the complete information about probability distributions for the whole time period of evolution. In SDEs, since one sample only provides one out of the many possible trajectories, a complete range estimation for variation requires a very large number of samples. FPEs provide the global picture of distributions and are solved typically by path integral methods. Yet, all possible states need to be known during the solving process. The memory requirement to store transition matrix that captures the dynamics in a fine-grained state space can be-

come prohibitive. Additionally, the time step is required to be small enough for accurate estimation of short-time transition probabilities in the path integral methods.

Recently, a continuous-time quantum walk approach was proposed to simulate stochastic drift-diffusion processes in one-dimensional (1-D) lattice space (Wang, 2013). With a novel formulation that combines quantum and random diffusions in the simulation algorithm, drastic acceleration can be achieved by the use of non-local correlation in quantum systems. This acceleration is particularly useful in simulating complex dynamic systems such as in stochastic resonance problems. The numerical results showed that the formulation provides an effective approach to simulate stochastic drift-diffusion processes.

In this paper, the quantum walk based diffusion simulation formulation is generalized to simulate processes in two- or higher-dimensional space. A new quantum operator is proposed for drift-diffusion processes on graphs. By combining quantum walks in the topological space and drift-diffusion in the Euclidean space, simulation can be accelerated.

In the remainder of the paper, Section 2 provides the background of numerical methods of solving FPEs and quantum walks. Section 3 summarizes the 1-D continuous-time quantum walk formulation to accelerate the stochastic drift-diffusion processes. In Section 4, the 1-D formulation is generalized to high-dimensional diffusion problems with quantum walks on graphs. In Section 5, a numerical example is given to demonstrate the effectiveness and efficiency of the proposed approach.

2 Background

2.1 Solving Fokker-Planck Equations for Stochastic Diffusions

Stochastic drift-diffusion processes can be generally modeled by FPEs, which describe the time evolution of probability density functions in the state space. Various numerical methods to solve FPEs have been developed, including Monte Carlo (Ermak and Buckholz, 1980), finite element (Masud and Bergman, 2005), finite difference (Park and Petrosian, 1996), spectral approximation by polynomials (Wei, 1999; Spanos et al., 2007), and path integral (Haken, 1975).

In particular, the path integral method has been shown as a simple yet accurate approach. Wehner and Wolfer (Wehner and Wolfer, 1983) used a short-time transition probability density matrix to approximate the evolution of drift-diffusion processes. To improve numerical efficiency and accuracy, Naess et al. (Naess and Johnsen, 1993; Naess and Moe, 2000) developed a B-spline interpolation approach where continuous probability density functions are approximated based upon limited discrete evaluations such that the error reduction speed is increased to $O(\tau)$ with time step size τ. Spencer and Bergman (Spencer and Bergman, 1993) solved the equation by direct polynomial interpolations in the state space. Santoro et al. (Di Paola and Santoro, 2008; Pirrotta and Santoro, 2011) extended the path integral approach for systems under Gaussian white noise perturbation as in the classical Fokker-Planck equation to the Kolmogorov-Feller equation under Poisson white noise. Kougioumtzoglou and Spanos (Kougioumtzoglou and Spanos, 2012) developed an analytical approach to calculate distributions based on a variational formulation for nonlinear oscillation problems, instead of using short time steps as in path integrals, to improve the computational efficiency. Narayanan and Kumar (Narayanan and Kumar, 2012) used Gauss-Legendre integration to approximate non-Gaussian transition probability densities. Di Paola et al. (Cottone and Di Paola, 2009; Di Matteo et al., 2014) recently developed a fractional calculus approach to solve stochastic dynamics problems based on fractional complex moments.

2.2 Quantum Walks

In this paper, a new formulation to simulate stochastic diffusions based on quantum walks is proposed. Quantum walk can be considered as a quantum version of the classical random walk, where a stochastic system is modeled in terms of probability amplitudes instead of probabilities. In random walk, the system's state $\mathbf{x}$ at time t is described by a probability distribution $p(\mathbf{x}, t)$. The system evolves by transitions. The state distribution after a time period of τ is $p(\mathbf{x}, t+\tau) = T(\tau)p(\mathbf{x}, t)$ where $T(\tau)$ is the transition operator. In quantum walk, the system's state is described by the complex-valued am-

plitude $\psi(\mathbf{x},t)$. Its relationship with the probability is $\psi^*\psi = |\psi|^2 = p$. The system evolution then is modeled by $\psi(\mathbf{x},t+\tau) = U(\tau)\psi(\mathbf{x},t)$ with U being a unitary and reversible operator. In quantum walks, probability is replaced by amplitude and Markovian dynamics is replaced by unitary dynamics.

Similar to random walks, there are discrete-time quantum walks and continuous-time quantum walks. The study of discrete-time quantum walks started from 1990s (Meyer, 1996; Ambainis et al., 2001) in the context of quantum algorithm and computation (Kempe, 2003; Kendon, 2007; Konno, 2008). Although the term, continuous-time quantum walk, was introduced more recently (Farhi and Gutmann, 1998), the research of the topic can be traced back much earlier in studying the dynamics of quantum systems, particularly in the path integral formulation of quantum mechanics generalized by Feynman (Feynman, 1948) in 1940's. The relationship between the discrete- and continuous-time quantum walks was also studied. The two models have similar speed performance and intrinsic relationships. The convergence of discrete-time quantum walks toward continuous-time quantum walks has been demonstrated (Strauch, 2006; Childs, 2010).

3 Quantum Walks in One-Dimensional Lattice Space

The quantum diffusion is described by the Schrödinger equation

$$i\frac{d}{dt}\psi(\mathbf{x},t) = \hat{H}(t)\psi(\mathbf{x},t) \tag{1}$$

where $\hat{H}(t)$ is the Hamiltonian. Path integral is a classical approach to solve the quantum dynamics problem. To construct the unitary operator U that describes quantum state transitions, a general *functional integral* (Farhi and Gutmann, 1992)

$$F_{jk} := \int dq_{jk} e^{-i\int_{t_0}^{t_0+\tau} W_{q(s)}ds} \prod_{l\to m} e^{i\theta_{ml}} \tag{2}$$

for a path from state x_k to state x_j is applied. A *path* $q(s)$ is defined as a functional mapping from time s to the state space. For instance, $q(t_0) = x_k$ and $q(t_0+\tau) = x_j$ represent the transitional path from state x_k to state x_j during a time period of τ. $\int_{t_0}^{t_0+\tau} W_{q(s)}ds$ gives the overall probability of all possible paths from x_k at time t_0 to x_j at time $t_0+\tau$. $e^{-i\int_{t_0}^{t_0+\tau} W_{q(s)}ds}$ can be regarded as the *weight* of transition from x_k to x_j. $\prod_{l\to m} e^{i\theta_{ml}}$ is the *total phase shift factor* for all jumps in transition from x_k to x_j, where each of $e^{i\theta_{ml}}$ corresponds to the phase shift for one of the jumps during the transition. Here, dq_{jk} is the probabilistic measure on the path from x_k to x_j, which is analogous to continuous-time Markov chain model. The probabilistic measure for one path from state 0 to $n\Delta$ that has l left jumps is (Wang, 2013)

$$dq_{n,0}^{(l)} = \frac{e^{-b\tau/(2\Delta^2)}(\frac{b\tau}{2\Delta^2})^l}{l!}\frac{e^{-b\tau/(2\Delta^2)}(\frac{b\tau}{2\Delta^2})^{n+l}}{(n+l)!} \tag{3}$$

Continuous-time quantum walks can be used to model the quantum drift-diffusion and random drift-diffusion processes in 1-D lattice space with different functional integrals, described as follows.

3.1 Quantum Drift-Diffusion Process

The quantum drift-diffusion process is described by

$$i\frac{\partial}{\partial t}\psi(x,t) = -\frac{b}{2}\frac{\partial^2}{\partial x^2}\psi(x,t) - iV(x,t)\psi(x,t) \tag{4}$$

where b is the diffusion coefficient and V is the potential function. For a transition with n steps away from the initial state for a total period τ, the weight for the functional integral in Eq.(2) can be calculated as

$$e^{-i\sum_l W_l\tau_l} = e^{-i\sum_l[\frac{b}{\Delta^2}+i(\frac{b}{\Delta^2}-V_l)]\tau_l} \approx e^{(1-i)\frac{b}{\Delta^2}\tau - V_n\tau}$$

where V_n denotes the potential at the final state and $\sum_l \tau_l = \tau$. With the probabilistic measure as in Eq.(3), the complete functional integral for quantum drift-diffusion processes is (Wang, 2013)

$$F_{n,0} = i^n e^{-ib\tau/\Delta^2 - V_n\tau} J_n(\frac{b\tau}{\Delta^2}) \tag{5}$$

where $J_n(y)$ is the *Bessel function of first kind* with integer order n and input y ($y \geq 0$). Notice that for diffusion processes without drift, the potential V_n in Eq.(5) is a constant or zero.

3.2 Random Drift-Diffusion Process

The one-dimensional random drift-diffusion process is described by an imaginary-time quantum system as

$$-\frac{\partial}{\partial t}\psi(x,t) = -\frac{b}{2}\frac{\partial^2}{\partial x^2}\psi(x,t) - iV(x,t)\psi(x,t) \quad (6)$$

where $V(x,t)$ is the potential function. Here, the weight in Eq.(2) becomes $e^{-i\sum_l W_l\tau_l}$ where τ_l is the duration that the system stays at state l during the transition. If the total duration of transition $\tau = \sum_l \tau_l$ is small, then the weight can be numerically approximated as $e^{-iW_n\tau}$ where W_n is the transition rate corresponding to the final state at time $t_0+\tau$.

With the same probabilistic measure as in Eq.(3), the final functional integral for random drift-diffusion processes is (Wang, 2013)

$$F_{n,0} = \sum_{l=0}^{\infty} e^{-b\tau V_n} dq_{ji}^{(l)} = e^{-(V_n+b/\Delta^2)\tau} I_n(\frac{b\tau}{\Delta^2}) \quad (7)$$

where V_n is the potential corresponding to the final state at time $t_0+\tau$, and $I_n(y)$ is the *modified Bessel function of first kind* with integer order n and input y ($y \geq 0$).

4 Quantum-Random Diffusion on Graphs

4.1 Quantum Diffusion on Graphs

Quantum diffusion on graphs based on CTQW formulation can be computed by spectral analysis. Suppose that the adjacency matrix of a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is H, where $\mathcal{V} = \{v_i\}$ is a set of nodes and $\mathcal{E} = \{(v_i, v_j)\}$ is a set of edges. The elements of the adjacency matrix H are defined as $H_{ij} = 1$ if $(v_i, v_j) \in \mathcal{E}$, $H_{ij} = 0$ otherwise, and $H_{ii} = 0$ for $i, j = 1, 2, \ldots$. We use $\partial(v_i, v_j)$ to denote the shortest graph distance between nodes v_i and v_j as a natural number. For instance, $\partial(v_i, v_i) = 0$. $\partial(v_i, v_j) = 1$ if there exists an edge $(v_i, v_j) \in \mathcal{E}$.

Let Γ be a K-dimensional Hilbert space with an orthonormal basis $\{\phi_0, \phi_1, \ldots, \phi_{K-1}\}$. We define a *creation operator* H^+, an *annihilation operator* H^-, and a *conservation operator* H° such that (Hora and Obata, 2007)

$$\begin{aligned} H^+\phi_k &= \sqrt{\omega_{k+1}}\phi_{k+1} \ (k = 0, 1, 2, \ldots) \\ H^-\phi_k &= \sqrt{\omega_k}\phi_{k-1} \ (k = 1, 2, \ldots) \\ H^-\phi_0 &= 0 \\ H^\circ\phi_k &= \alpha_{k+1}\phi_k \ (k = 0, 1, 2, \ldots) \end{aligned} \quad (8)$$

A pair of sequences $(\{\omega_k\}, \{\alpha_k\})$ is called *Jacobi parameters* or *Jacobi coefficients* with $\{\omega_k\}$ being a *Jacobi sequence*.

The adjacency matrix is decomposed as $H = H^+ + H^- + H^\circ$, as a process of stratification. Its interpretation in quantum walks on graphs is as follows. By specifying a reference or origin node v_0 in the graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, we decompose the nodes in $\mathcal{G}$ into strata as $\mathcal{V} = \bigcup \mathcal{V}_k$, where $\mathcal{V}_k = \{v \in \mathcal{V} : \partial(v, v_0) = k\}$ is the stratified set of nodes that has a shortest graph distance of k to the origin node v_0.

The orthonormal basis in Eq.(8) can be constructed as

$$\phi_k = \frac{1}{\sqrt{|\mathcal{V}_k|}} \sum_{v \in \mathcal{V}_k} |k, v\rangle \quad (9)$$

where $|k, v\rangle$ denotes the eigenket of vertex v in the k-th stratum of nodes $\mathcal{V}_k$. Then the elements of H^+, H^-, and H° are defined as follows. For $v_i \in \mathcal{V}_k$, $H^+_{ji} = H_{ji}$ if $v_j \in \mathcal{V}_{k+1}$, otherwise $H^+_{ji} = 0$. $H^-_{ji} = H_{ji}$ if $v_j \in \mathcal{V}_{k-1}$, otherwise $H^-_{ji} = 0$. $H^\circ_{ji} = H_{ji}$ if $v_j \in \mathcal{V}_k$, otherwise $H^\circ_{ji} = 0$. Therefore, H^+, H^-, and H° specify the adjacency relations between the nodes of the current stratum and those of the 'forward' stratum, between of the current and of the 'backward', as well as within the current stratum, respectively. Then the diffusion process on a graph can be modeled as CTQWs on the graph starting from v_0. The propagation is through the strata of nodes.

The Jacobi coefficients capture the edge valences between strata. For $j \in \mathcal{V}_{k+1}$, $\sqrt{\omega_{k+1}} = \kappa^-_j\sqrt{|\mathcal{V}_{k+1}|/|\mathcal{V}_k|}$ where $\kappa^-_j = |\{v \in \mathcal{V}_k : \partial(v, v_j) = 1\}|$. For $i \in \mathcal{V}_k$, $\alpha_{k+1} = \kappa^\circ_i$ where $\kappa^\circ_i = |\{v \in \mathcal{V}_k : \partial(v, v_i) = 1\}|$. That is, ω_k's characterize the inter-strata valence whereas α_{k+1} represents the valence inside the k-th stratum.

With Gram-Schmidt orthogonalization, polynomi-

als $\{P_k(\xi)\}_{k=0}^{\infty}$ can be obtained as

$$\begin{aligned} &P_0(\xi) = 1, \\ &P_1(\xi) = \xi - \alpha_1, \\ &xP_k(\xi) = P_{k+1}(\xi) + \alpha_{n+1}P_n(\xi) + \omega_k P_{k-1}(\xi) \end{aligned} \quad (10)$$

where $k = 1, 2, \ldots$. Based on Eqs.(8) and (18), given a probability measure μ defined by the moments

$$\langle e_0, (H^+ + H^- + H^\circ)^m e_0 \rangle = \int_{-\infty}^{+\infty} \xi^m \mu(\xi) d\xi \quad (m = 1, 2, \ldots) \quad (11)$$

we have

$$\langle \phi_k, H^m \phi_0 \rangle = \frac{1}{\sqrt{\omega_1 \omega_2 \ldots \omega_k}} \int_{-\infty}^{+\infty} \xi^m P_k(\xi) \mu(\xi) d\xi \quad (m = 1, 2, \ldots) \quad (12)$$

The functional integral for amplitude update at the k-th stratum for CTQW on the graph is

$$\begin{aligned} F_{k,0}(\tau) &= \langle \phi_k, e^{-iH\tau} \phi_0 \rangle \\ &= \frac{1}{\sqrt{\omega_1 \omega_2 \ldots \omega_k}} \int_{-\infty}^{+\infty} e^{-i\xi\tau} P_k(\xi) \mu(\xi) d\xi \end{aligned} \quad (13)$$

4.2 Quantum Drift-Diffusion on Graphs

Different from the above CTQWs on graphs, the quantum drift-diffusion process on graphs has an external potential field involved. Similar to Eq.(5), the proposed functional integral for quantum drift-diffusion processes in graphs is

$$\begin{aligned} &F_{k,0}(\mathbf{x}_n, \mathbf{x}_0, \tau) \\ &= \frac{e^{-iC(\mathbf{x}_n, \mathbf{x}_0, \tau) - V(\mathbf{x}_n, t)\tau}}{\sqrt{\omega_1 \omega_2 \ldots \omega_k}} \int_{-\infty}^{+\infty} e^{-i\xi\tau} P_k(\xi) \mu(\xi) d\xi \end{aligned} \quad (14)$$

where $V(\mathbf{x}, t)$ is the potential field in the configuration space and is associated with drift, $C(\mathbf{x}_n, \mathbf{x}_0, \tau)$ is the work of diffusion from node $\mathbf{x}_0$ to node $\mathbf{x}_n$, and t is the time.

To illustrate, a two-dimensional (2-D) Euclidean space $\chi = \{\mathbf{x} = (x, y)\}$ in the neighborhood of $\mathbf{x}_0 = (x_0, y_0)$ is discretized to $N_1 \times N_2$ nodes as a regular grid $\chi^d = \{\ldots, (x_0 - 1, y_0 - 1), (x_0 - 1, y_0), (x_0, y_0 - 1), (x_0, y_0), (x_0 + 1, y_0), (x_0, y_0 + 1), (x_0 + 1, y_0 + 1), \ldots\}$. A graph is formed with each edge connecting two spatially adjacent nodes. and partitioned into K subspaces $\{\chi_1^d, \ldots, \chi_K^d\}$ according to the distances. For instance, $\chi_1^d = \{(x_0 - 1, y_0), (x_0 + 1, y_0), (x_0, y_0 - 1), (x_0, y_0 + 1)\}$, and $\chi_2^d = \{(x_0 - 2, y_0), (x_0 - 1, y_0 - 1), (x_0 - 1, y_0 + 1), (x_0, y_0 - 2), (x_0, y_0 + 2), (x_0 + 1, y_0 - 1), (x_0 + 1, y_0 + 1), (x_0 + 2, y_0)\}$. The nodes $\chi_1^d, \ldots, \chi_K^d$ correspond to K strata in the graph.

Suppose that the diffusion matrix in the 2-D space is $\mathbf{B}(\mathbf{x}, t) \in \mathbb{R}^{2\times 2}$ and the drift vector is $\mathbf{A}(\mathbf{x}, t) \in \mathbb{R}^{2\times 1}$ for a 2-D problem. The relation between the drift vector and the potential function is $\mathbf{A} = [-\partial V/\partial x, -\partial V/\partial y]^T$. In the Euclidean space, the work of diffusion from node $\mathbf{x}_0$ to node $\mathbf{x}_n$ is calculated as

$$\begin{aligned} &C(\mathbf{x}_n, \mathbf{x}_0, \tau) \\ &= ((\mathbf{x}_n - \mathbf{x}_0 - \mathbf{A}\tau)^T \mathbf{B}^{-1} (\mathbf{x}_n - \mathbf{x}_0 - \mathbf{A}\tau))/(2\tau) \end{aligned} \quad (15)$$

4.3 Quantum-Random Drift-Diffusion in 2-D Space

The functional integral in Eq.(14) describes the process of quantum drift-diffusion in two or higher dimensional space. Similar to the one-dimensional case in Section 3.2, the random drift-diffusion process in 2-D space can be described with an imaginary-time quantum formulation. The proposed functional integral for random drift-diffusion processes is

$$\begin{aligned} &F_{k,0}(\mathbf{x}_n, \mathbf{x}_0, \tau) \\ &= \frac{e^{-C(\mathbf{x}_n, \mathbf{x}_0, \tau) - V(\mathbf{x}_n, t)\tau}}{\sqrt{\omega_1 \omega_2 \ldots \omega_k}} \int_{-\infty}^{+\infty} e^{-i\xi\tau} P_k(\xi) \mu(\xi) d\xi \end{aligned} \quad (16)$$

To build a graph to cover the 2-D space, a comb graph (Accardi et al., 2004) is chosen because it provides an effective structure yet with simple polynomials. The comb product of a backbone graph G_1 and a finger graph G_2 is obtained by grafting a copy of G_2 into each vertex of G_1 at G_2's reference vertex o, as shown in Fig. 1.

In the 2-D comb lattice in Fig. 2, the strata are indicated by the dashed lines, with respect to the

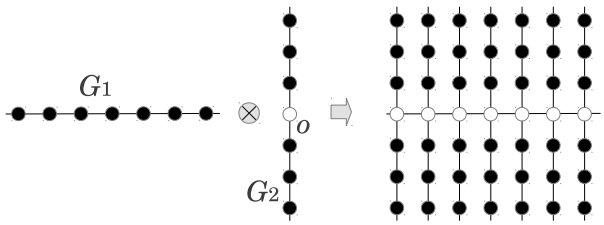

Figure 1: Comb product combines two 1-D lattices into a 2-D lattice

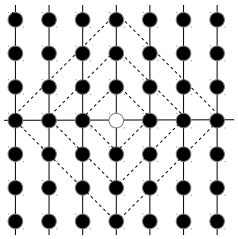

Figure 2: The strata in the 2-D comb lattice

reference node in white. The number of nodes in strata are $|\mathcal{V}_0| = 1$ and $|\mathcal{V}_k| = 4k$ $(k = 1, 2, \ldots)$. The Jacobi coefficients are $\omega_1 = 4$, $\omega_k = k/(k-1)$ $(k = 2, 3, \ldots)$, and $\alpha_k = 0$ $(k = 1, 2, \ldots)$. It has been shown that (Accardi et al., 2004; Jafarizadeh and Salimi, 2007)

$$\mu(\xi) = \frac{1}{\pi\sqrt{8-\xi^2}} \quad (2\sqrt{2} \leq \xi \leq -2\sqrt{2}) \tag{17}$$

Based on Eq.(18), we have

$$\begin{aligned} P_0(\xi) &= 1 \\ P_1(\xi) &= \xi \\ P_2(\xi) &= \xi^2 - 4 \\ P_{k+1}(\xi) &= xP_k(\xi) - k/(k-1)P_{k-1}(\xi) \ (k = 2, 3, \ldots) \end{aligned} \tag{18}$$

Then the functional integral in Eq.(16) can be calculated as

$$\begin{aligned} &F_{k,0}(\mathbf{x}_n, \mathbf{x}_0, \tau) \\ &= \frac{e^{-C(\mathbf{x}_n,\mathbf{x}_0,\tau)-V(\mathbf{x}_n,t)\tau}}{\sqrt{\omega_1\omega_2\ldots\omega_k}} \int_{-2\sqrt{2}}^{2\sqrt{2}} \frac{e^{-i\xi\tau}P_k(\xi)}{\pi\sqrt{8-\xi^2}} d\xi \end{aligned} \tag{19}$$

With the advantage of the strong non-local correlation in quantum diffusion, large step sizes can be taken during the simulation, which significantly accelerates the simulation of stochastic diffusion. Algorithm 1 shows the algorithm of simulating diffusion. The timing of simulation is based on the quantum walk time step τ_Q. A much shorter time step τ_R is used to perform one step of traditional path integral for probability distribution update. In other words, one step of quantum walk based on quantum operator U_Q is followed by one step of traditional path integral based on the short-time transition probability T_R in each iteration of the simulation.

Algorithm 1 The quantum walk algorithm to simulate stochastic drift-diffusion processes based on the formulation of quantum and random diffusions

1: $\psi = \psi_0(\mathbf{x})$;
2: $t = 0$;
3: **while** $t < T$ **do** ▷ main iterations of search
4: update quantum operator $U_Q = F(\tau_Q, \mathbf{A}, \mathbf{B}, \mathbf{V}, \mathbf{x}, t)$ by Eq.(16);
5: $|\psi\rangle = U_Q|\psi\rangle$;
6: $P = \langle\psi|\psi\rangle$;
7: update short-time transition probability $T_R = C(\tau_R, \mathbf{A}, \mathbf{B}, \mathbf{x}, t)$ by Eq.(15)
8: $P = T_R P$;
9: output probability P at time t;
10: $t = t + \tau_Q$;
11: **end while**

5 A Numerical Example

In this section, a numerical example is used to demonstrate the new quantum walk based diffusion simulation method. The stochastic resonance phenomenon is a nonlinear response of a system with sinusoidal inputs simultaneously subject to noise, where the system oscillates between states. To simulate stochastic resonance using traditional path integral approaches, small time step sizes need to be chosen so that the simulated paths represent the actual dynamics in the physical system. In contrast, quantum walk based drift-diffusion simulation can use much larger step sizes so that the simulation can be accelerated.

The simulated system is described by

$$\begin{aligned}\frac{\partial}{\partial t}p(x_1,x_2,t) = &-\frac{\partial}{\partial x_1}(g_1(x_1,x_2)p(x_1,x_2,t)) \\ &-\frac{\partial}{\partial x_2}(g_2(x_1,x_2)p(x_1,x_2,t)) \\ &+D\frac{\partial^2}{\partial x_2^2}p(x_1,x_2,t) \qquad (20)\end{aligned}$$

where the position x_1 and velocity x_2 represent the system's state that evolves along time t. Functions

$$\begin{aligned}g_1(x_1,x_2) &= x_2 \\ g_2(x_1,x_2,t) &= x_1 - 2\zeta\epsilon x_2 - a_0\sin(2\pi f_0 t)\end{aligned}$$

define the drifting coefficients, where ζ and ϵ damping parameters, a_0 is the oscillation coefficient, and f_0 is the oscillation frequency. The corresponding potential function is

$$V(x_1,x_2,t) = -x_1x_2 - \zeta(1-\epsilon x_2^2) + a_0\sin(2\pi f_0 t)x_2$$

In this example, the values of the parameters are $\zeta = 0.5$, $\epsilon = 1.0$, $D = 1.0$, $a_0 = 20$, and $f_0 = 0.1$. The drift vector is $\mathbf{A} = [g_1(x_1,x_2), g_2(x_1,x_2,t)]^T$ and the diffusion matrix is

$$\mathbf{B} = \begin{bmatrix} D & 0 \\ 0 & Dx_2^2 \end{bmatrix}$$

In the simulation, the step size for quantum walks is $\tau_Q = 1.0$ whereas the one in the path integral method is $\tau_R = 0.1$. For comparison, the system is also simulated by the path integral method with a time step size of $\tau = 0.1$. Figs. 3 and 4 show the probability evolutions computed by traditional path integral and the proposed CTQW based methods respectively. The system oscillates between two stable states, which appear at times $t = 5$ and $t = 10$ respectively. A 'rotational' motion appears during the dynamic transition process. Figs. 5 and 6 compare the respective contour lines of probability densities by the two methods.

6 Concluding Remarks

In this paper, a new continuous-time quantum walk formulation is developed to simulate stochastic drift-diffusion processes in two- or higher-dimensional spaces. The random drift-diffusion process is modeled as the dynamics of imaginary-time quantum systems. The new simulation algorithm combines continuous-time quantum walk on graphs with path integral in Euclidean space. The formulation is generic and applicable to diffusions when potential functions are available. The advantages of the proposed quantum walks based approach is the drastic quantum acceleration by choosing larger time step sizes. The acceleration is particularly attractive when simulating stochastic resonance, where the system dynamically oscillates between stable states. The nonlocal quantum tunneling effect help the simulation based on large step sizes without the issue of possibly missing stable states in traditional path integral approaches. If the algorithm is implemented in the actual quantum computer, the additional advantage is the efficiency of representing large state space by qubits.

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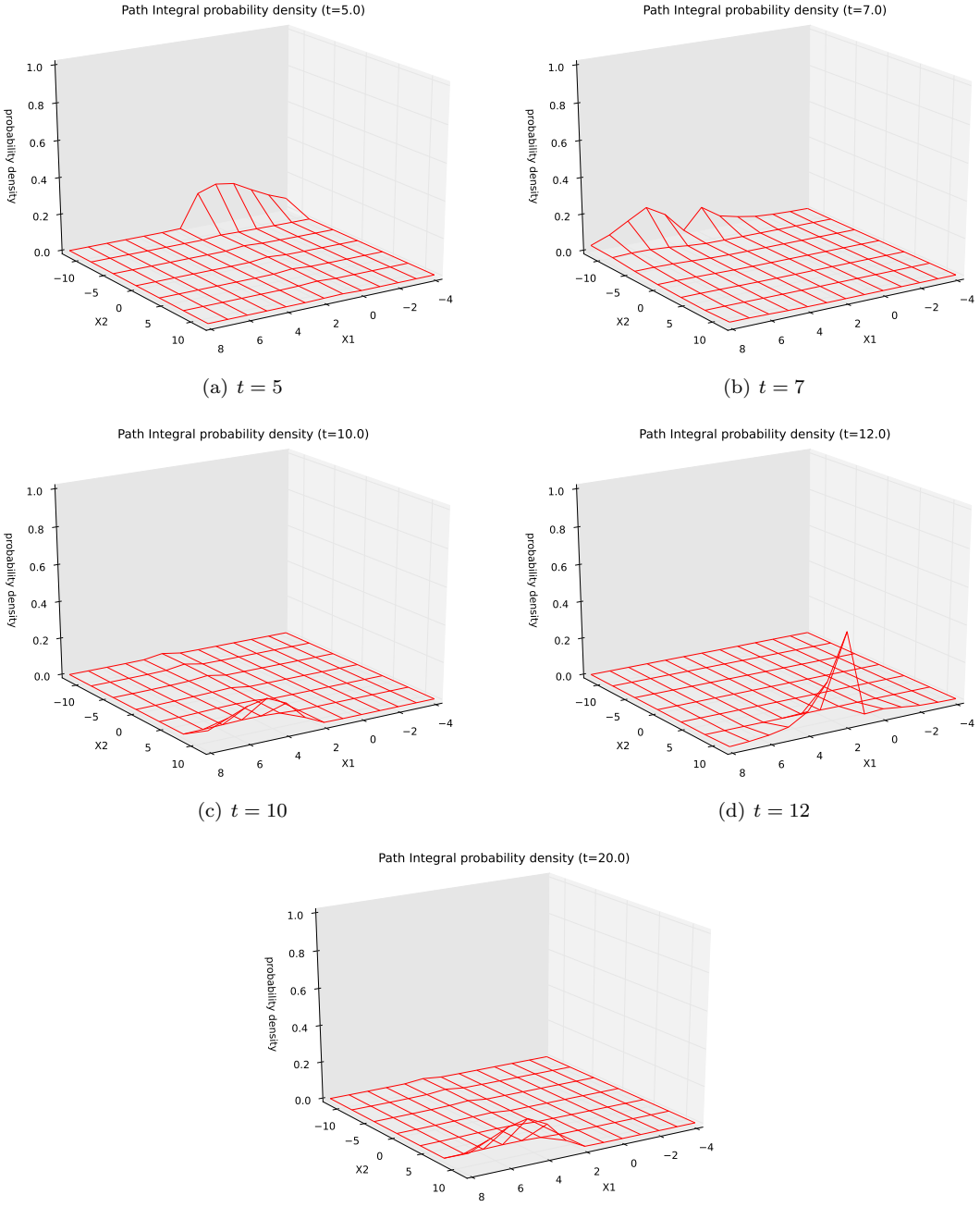
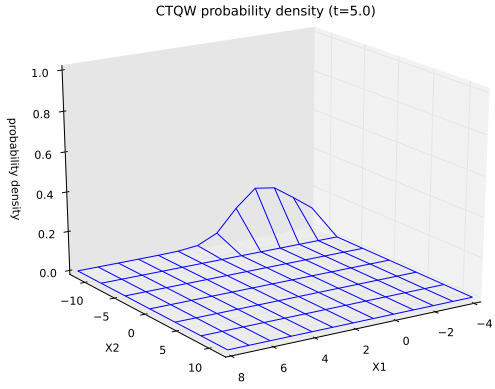


(a) $t = 5$ (b) $t = 7$

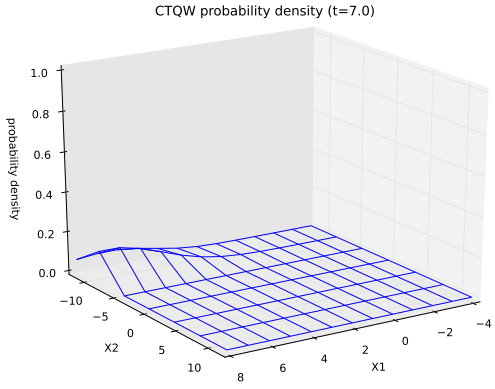
(c) $t = 10$ (d) $t = 12$

(e) $t = 20$

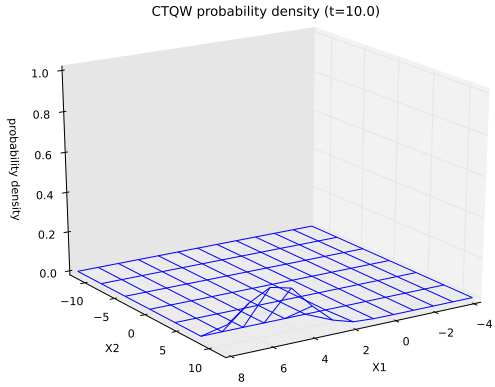
Figure 3: Evolution of probability density simulated by the path integral method



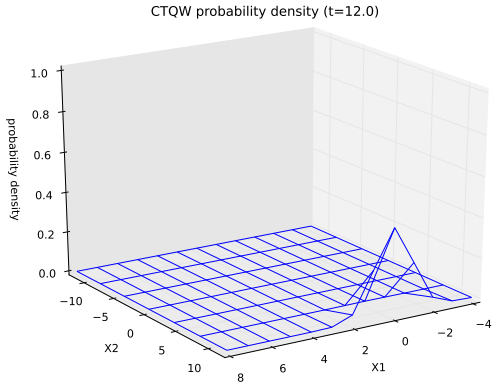
(a) $t = 5$



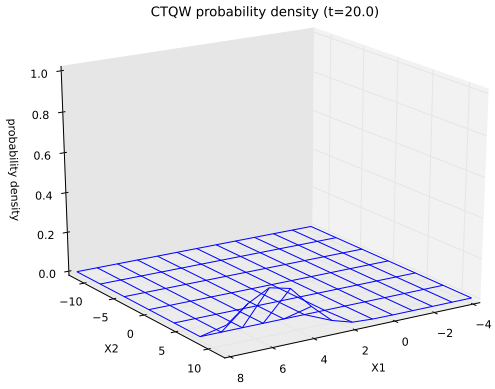
(b) $t = 7$



(c) $t = 10$

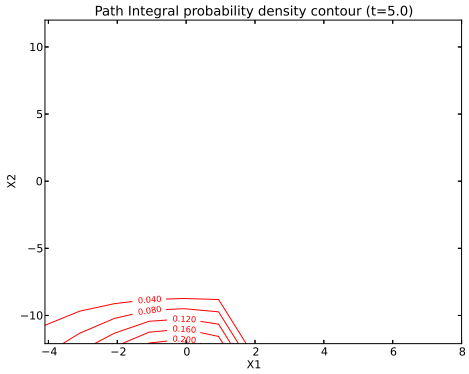


(d) $t = 12$

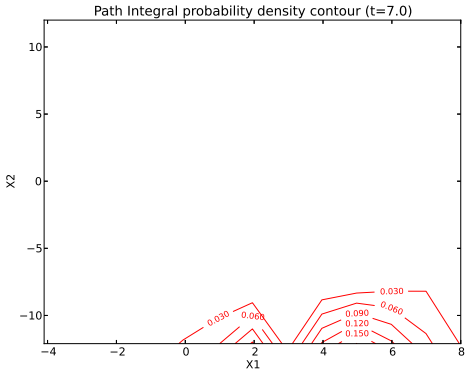


(e) $t = 20$

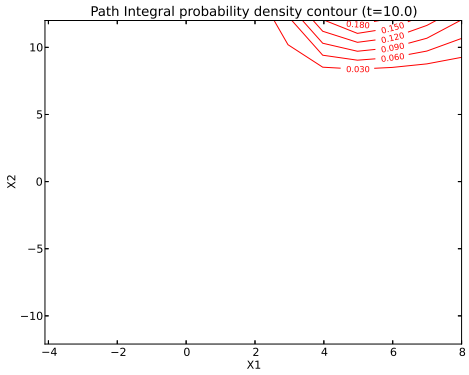
Figure 4: Evolution of probability density simulated by the CTQW method



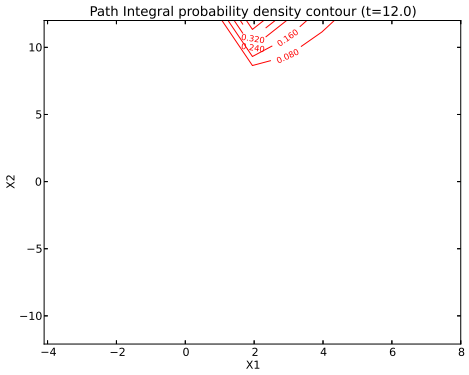
(a) $t = 5$



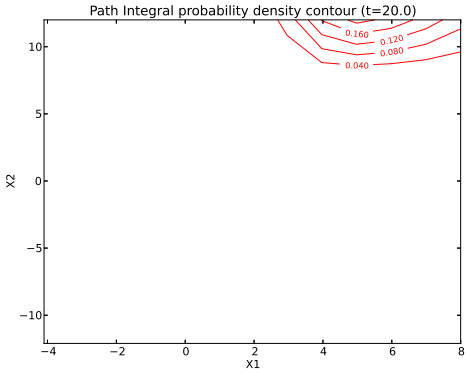
(b) $t = 7$



(c) $t = 10$

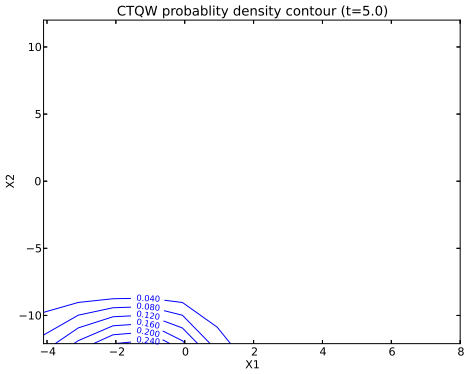


(d) $t = 12$

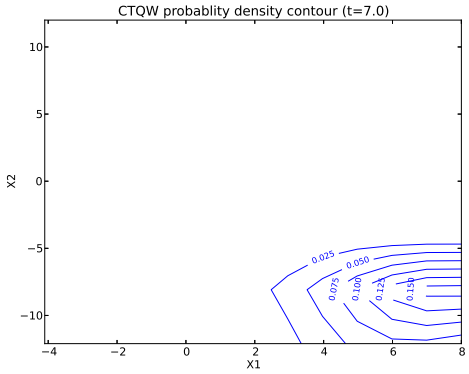


(e) $t = 20$

Figure 5: Contours of probability density simulated by the path integral method



(a) $t = 5$



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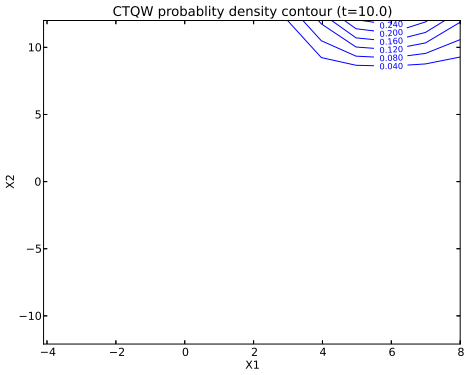
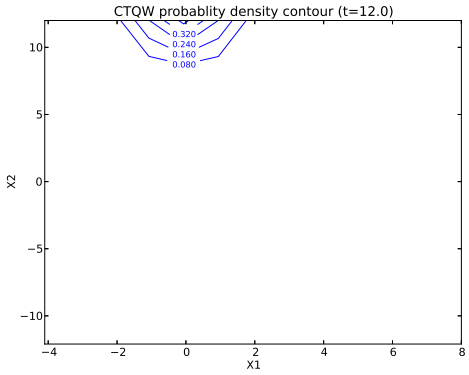
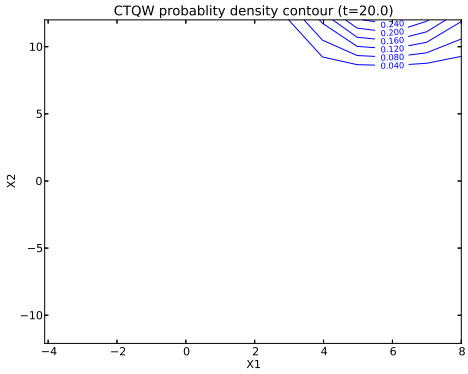


(c) $t = 10$



(d) $t = 12$



(e) $t = 20$

Figure 6: Contours of probability density simulated by the CTQW method

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