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ACCELERATING STOCHASTIC DYNAMICS SIMULATION WITH CONTINUOUS-TIME QUANTUM WALKS

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ABSTRACT

Stochastic diffusion is a general phenomenon observed in various national and engineering systems. It is typically modeled by either stochastic differential equation (SDE) or Fokker-Planck equation (FPE), which are equivalent approaches. Path integral is an accurate and effective method to solve FPEs. Yet, computational efficiency is the common challenge for path integral and other numerical methods, include time and space complexities. Previously, one-dimensional continuous-time quantum walk was used to simulate diffusion. By combining quantum diffusion and random diffusion, the new approach can accelerate the simulation with longer time steps than those in path integral. It was demonstrated that simulation can be dozens or even hundreds of times faster. 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 are computed efficiently by spectral analysis. The efficiency of the new method is demonstrated with stochastic resonance problems.

1 INTRODUCTION

Stochastic diffusion processes are universally observed in various physical, chemical, biological and economical systems. In engineering applications, we need to simulate the diffusion phenomena and design systems and device with desirable 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 processes are typically modeled with stochastic differential equations (SDEs) or Fokker-Planck equations (FPEs). These two approaches are equivalent in describing the drift-diffusion processes. SDEs simulate systems under noises by considering the possible trajectories of the systems as a result of Wiener process, whereas FPEs describe the behaviors by modeling the time evoluation of the probability distributions of possible system states .

Except for a few simple ones with closed-form solutions or using backward approaches, solving SDEs typically relies on the Monte Carlo sampling of system trajectories, i.e. the solutions of ordinary differential equations, with randomly generated inputs to describe the stochastic processes. A large number of samples thus need to be generated and output statistics are collected to draw meaningful conclusions. Obviously large sample sizes make solving SDEs inefficient. In contrast, a FPE captures the dynamics of the probability density for all possible states at a time and the solution as probability densities is found deterministically. The evolution process of the overall probability distribution is described by the equation.

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 the path integral like methods. The path integral method [1] is proven to be a simple yet accurate approach

to solve FPEs. Nevertheless, the approach has two limitations. First, all possible states need to be known during the solving process. The memory requirement to store transition matrix that captures the dynamics in a very fine-grained state space can become prohibitive. Second, the time step is required to be small enough for accurate estimation of the so-called short-time transition probabilities in the path integral methods. Thus the simulation will be slow and expensive for systems that require long time periods of simulation. Other alternative methods to solve FPEs such as Monte Carlo, finite element, finite difference, spectral approximation similarly face the above two space and time limitations.

Recently, a novel continuous-time quantum walk based simulation formulation was proposed to simulate stochastic drift-diffusion processes in one-dimensional lattice space [2]. The new formulation is based on the concept that a quantum drift-diffusion process is typically described by the Schrödinger equation as a real-time quantum system, whereas a stochastic drift-diffusion process is modeled as an imaginary-time quantum system, as an extension. The main idea of the hybrid approach is to combine quantum diffusion with stochastic diffusion in simulating stochastic dynamics. Quantum diffusion is modeled with continuous-time quantum walks, whereas stochastic diffusion with random walks. Quantum walk has the special property of quantum tunneling that captures long-range spatial correlation effect. As a result, continuous-time quantum walk with long time steps can be chosen in simulating the dynamics. We combine quantum walks with stochastic diffusion so that the simulation of stochastic dynamics can be accelerated compared to the traditional path integral method. The acceleration is achieved by choosing long time steps of continuous-time quantum walks. In each iteration of simulation, a long time step of quantum walk is applied, followed by a short time step of random walk as stochastic diffusion. This acceleration is particularly helpful in nonlinear dynamics system such as stochastic resonance.

To generalize the proposed quantum walks based simulation to high-dimensional systems, a graph-based formalism is proposed in this paper. Multi-dimensional lattice structures with graph representation can be constructed by a comb product operation. The purpose is to construct graphs such that the topological distance from a source node to all other nodes can be easily tracked. Then the diffusion on graphs can be modeled based on the topological distance. A new quantum walk operator on graphs thus is constructed based on functional decomposition with respect to the stratified layers of nodes according to the topological distances.

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 [3], finite element [4], finite difference [5], spectral approximation by characteristic functions [6], polynomials [7, 8], and complex fractional moments [9], and path integral [1].

In particular, the path integral method has been shown as a simple yet accurate approach. Wehner and Wolfer [10] 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. [11, 12] 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 [13] solved the equation by direct polynomial interpolations in the state space. Di Paola and Santoro [14] 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 [15] 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 [16] used Gauss-Legendre integration to approximate non-Gaussian transition probability densities.

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 the 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 the quantum walk, the system's state is described by the complex-valued amplitude $\psi(\mathbf{x},t)$. Its relationship with the probability is $\psi^*\psi = |\psi|^2 = p$. The system evolution then is modeled by the quantum walk $\psi(\mathbf{x},t+\tau) = U(\tau)\psi(\mathbf{x},t)$ 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 [17, 18] in the context of quantum algorithm and computation [19–21]. Although the term, continuous-time quantum walk, was introduced more recently [22], 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 [23] 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 [24, 25].

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 $H(t)$ is the Hamiltonian and $i = \sqrt{-1}$. Continuous-time quantum walks in one-dimensional (1-D) space can be formulated to model the quantum drift-diffusion process, described by

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

where b is the diffusion coefficient and $V(x,t)$ is the potential function. 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* [26]

$$F_{jk} := \int dq_{jk} e^{-i\int_{t_0}^{t_0+\tau} W_{q(s)}ds} \prod_{l\to m} e^{i\theta_{ml}} \tag{3}$$

for a path from state x_k to state x_j is applied. 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. 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.

Similar to the classical Chapman-Kolmogorov equation of state transitions, a transition rate from state x_k to state x_j at time t in terms of probability amplitude is

$$\rho_{jk}e^{i\theta_{jk}} := -i\langle x_j|H(t)|x_k\rangle \tag{4}$$

where ρ_{jk} is the magnitude of transition rate and θ_{jk} is the phase. Then the magnitude of leaving state x_k is

$$\rho_k := \sum_{k\neq j}\rho_{jk} \tag{5}$$

and the overall transition rate for state x_k is determined by

$$W_k := \langle x_k|H(t)|x_k\rangle + i\rho_k \tag{6}$$

The elements of the Hamiltonian matrix $\hat{H}$ for 1-D lattice space that has integer indices and the spacing Δ are given by

$$\langle j|\hat{H}|k\rangle = -\frac{b}{2\Delta^2}\delta_{j,k-1} + (\frac{b}{\Delta^2} - iV_k)\delta_{j,k} - \frac{b}{2\Delta^2}\delta_{j,k+1} \tag{7}$$

where $\delta_{j,k}$ is the Kronecker delta, and the states are simply denoted by integers as $x = \ldots, -2, -1, 0, 1, 2, \ldots$.

For a transitional path with $k \neq j$,

$$\begin{aligned}\rho_{jk} &= \frac{b}{2\Delta^2}[\delta_{j,k-1} + \delta_{j,k+1}]\\ e^{i\theta_{jk}} &= i\\ \rho_k &= \rho_{k-1,k} + \rho_{k+1,k} = \frac{b}{\Delta^2}\\ W_k &= \frac{b}{\Delta^2} - iV_k + i\frac{b}{\Delta^2}\end{aligned}$$

Consider that the 1-D transitional paths are memoryless and the transition rate is $b/(2\Delta^2)$ per unit time. The numbers of jumps to the left or right direction within a time period follows a Poisson distribution. That is, the probability that there are l jumps to the left for time τ is $e^{-b\tau/(2\Delta^2)}(b\tau/(2\Delta^2))^l/l!$. Similarly it is $e^{-b\tau/(2\Delta^2)}(b\tau/(2\Delta^2))^r/r!$ for r jumps to the right. Assuming the final state is at n steps away and on the right to the initial state, $r-l=n$. The probabilistic measure dq_{jk} in Eq.(3) for one path from state 0 to $n\Delta$ that has l left jumps is

$$dq_{n,0}^{(l)} = \frac{e^{-b\tau/(2\Delta^2)}(b\tau/(2\Delta^2))^l}{l!}\frac{e^{-b\tau/(2\Delta^2)}(b\tau/(2\Delta^2))^{n+l}}{(n+l)!} \tag{8}$$

For a transition with n steps away from the initial state for a total period τ, the weight for the functional integral in Eq.(3) 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.(8), the complete functional integral for quantum drift-diffusion processes is [27]

$$F_{n,0} = i^n e^{-ib\tau/\Delta^2 - V_n\tau}J_n(\frac{b\tau}{\Delta^2}) \tag{9}$$

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.(9) is a constant or zero.

3.1 Random Drift-Diffusion Process

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

$$-\frac{\partial}{\partial t}\psi(x,t) = -\frac{b}{2}\frac{\partial^2}{\partial x^2}\psi(x,t) - iV(x,t)\psi(x,t) \tag{10}$$

where $V(x,t)$ is the potential function. Here, the weight in Eq.(3) 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.(8), the final functional integral for random drift-diffusion processes is [27]

$$F_{n,0} = \sum_{l=0}^{\infty} e^{-b\tau V_n} dq_{ji}^{(l)} = e^{-(V_n+b/\Delta^2)\tau} I_n\left(\frac{b\tau}{\Delta^2}\right) \tag{11}$$

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 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 [28]

$$\begin{aligned} H^+\phi_k &= \sqrt{\omega_{k+1}}\phi_{k+1} \ (k = 0, 1, 2, \ldots) \\ H^-\phi_k &= \sqrt{\omega_k}\phi_{k-1} \ (k = 1, 2, \ldots), \ H^-\phi_0 = 0 \\ H^\circ\phi_k &= \alpha_{k+1}\phi_k \ (k = 0, 1, 2, \ldots) \end{aligned} \tag{12}$$

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 $H = H^+ + H^- + H^\circ$. Its interpretation in quantum walks on graphs is by stratification 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.(12) can be constructed as

$$\phi_k = \frac{1}{\sqrt{|\mathcal{V}_k|}} \sum_{v \in \mathcal{V}_k} |k, v\rangle \tag{13}$$

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

$$\begin{aligned} &P_0(\xi) = 1, \\ &P_1(\xi) = \xi - \alpha_1, \\ &xP_k(\xi) = P_{k+1}(\xi) + \alpha_{n+1}P_n(\xi) + \omega_k P_{k-1}(\xi) \ (k = 1, 2, \ldots) \end{aligned} \tag{14}$$

Based on Eqs.(12) and (14), given a probability measure μ defined by the moments

$$\langle e_0, (H^+ + H^- + H^\circ)^m e_0\rangle = \int_{-\infty}^{+\infty} \xi^m \mu(\xi) d\xi \ (m = 1, 2, \ldots) \tag{15}$$

we have

$$\langle \phi_k, H^m \phi_0\rangle = \frac{1}{\sqrt{\omega_1\omega_2\ldots\omega_k}} \int_{-\infty}^{+\infty} \xi^m P_k(\xi)\mu(\xi)d\xi \ (m = 1, 2, \ldots) \tag{16}$$

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

$$F_{k,0}(\tau) = \langle \phi_k, e^{-iH\tau}\phi_0\rangle = \frac{1}{\sqrt{\omega_1\omega_2\ldots\omega_k}} \int_{-\infty}^{+\infty} e^{-i\xi\tau} P_k(\xi)\mu(\xi)d\xi \tag{17}$$

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. As an extension of Eq.(9), the functional integral for quantum drift-diffusion processes in graphs proposed here is

$$F_{k,0}(\mathbf{x}_n, \mathbf{x}_0, \tau) = \frac{e^{-iC(\mathbf{x}_n,\mathbf{x}_0,\tau) - V(\mathbf{x}_n,t)\tau}}{\sqrt{\omega_1\omega_2\ldots\omega_k}} \int_{-\infty}^{+\infty} e^{-i\xi\tau} P_k(\xi)\mu(\xi)d\xi \tag{18}$$

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

$$C(\mathbf{x}_n,\mathbf{x}_0,\tau) = ((\mathbf{x}_n - \mathbf{x}_0 - \mathbf{A}\tau)^T \mathbf{B}^{-1}(\mathbf{x}_n - \mathbf{x}_0 - \mathbf{A}\tau))/(2\tau) \quad (19)$$

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

The functional integral in Eq.(18) describes the process of quantum drift-diffusion in two or higher dimensional space. Similar to the one-dimensional case in Section 3.1, the random drift-diffusion process in 2-D space can be described with an imaginary-time quantum formulation. The proposed functional integral becomes

$$F_{k,0}(\mathbf{x}_n,\mathbf{x}_0,\tau) = \frac{e^{-C(\mathbf{x}_n,\mathbf{x}_0,\tau)-V(\mathbf{x}_n,t)\tau}}{\sqrt{\omega_1\omega_2\ldots\omega_k}} \int_{-\infty}^{+\infty} e^{-i\xi\tau} P_k(\xi)\mu(\xi)d\xi \quad (20)$$

To build a graph to cover the 2-D space, a comb graph [29] 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.

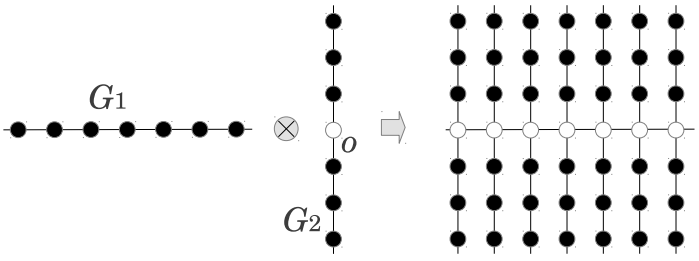

Figure 1. Comb product combines two 1-D lattices into a 2-D lattice

In the 2-D comb lattice in Fig. 2, the strata are indicated by the dashed lines, with respect to the 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 [29,30]

$$\mu(\xi) = \frac{1}{\pi\sqrt{8-\xi^2}} \quad (2\sqrt{2} \le \xi \le -2\sqrt{2}) \quad (21)$$

Based on Eq.(14), we have

$$\begin{aligned} P_0(\xi) &= 1 \\ P_1(\xi) &= \xi \\ P_2(\xi) &= \xi^2 - 4 \\ P_{k+1}(\xi) &= xP_k(\xi) - k/(k-1)P_{k-1}(\xi) \ (k = 2,3,\ldots) \end{aligned} \quad (22)$$

Then the functional integral in Eq.(20) can be calculated as

$$F_{k,0}(\mathbf{x}_n,\mathbf{x}_0,\tau) = \frac{e^{-C(\mathbf{x}_n,\mathbf{x}_0,\tau)-V(\mathbf{x}_n,t)\tau}}{\sqrt{\omega_1\omega_2\ldots\omega_k}} \int_{-2\sqrt{2}}^{2\sqrt{2}} \frac{e^{-i\xi\tau}P_k(\xi)}{\pi\sqrt{8-\xi^2}} d\xi \quad (23)$$

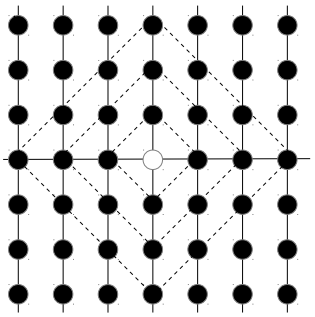

Figure 2. The strata in the 2-D comb lattice

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.

5 A NUMERICAL EXAMPLE

In this section, a numerical example of stochastic resonance is used to demonstrate the new quantum walk based diffusion simulation method. Stochastic resonance is a phenomenon that a nonlinear system is boosted by a combination of external periodic modulation (typically sinusoidal) and noise thus oscillates

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

$\psi = \psi_0(\mathbf{x})$;
$t = 0$;
while $t < T$ **do** ▷ main iterations of search
  update quantum operator $U_Q = F(\tau_Q, \mathbf{A}, \mathbf{B}, \mathbf{V}, \mathbf{x}, t)$ by Eq.(20);
  $|\psi\rangle = U_Q|\psi\rangle$;
  $P = \langle\psi|\psi\rangle$;
  update short-time transition probability $T_R = C(\tau_R, \mathbf{A}, \mathbf{B}, \mathbf{x}, t)$ by Eq.(19)
  $P = T_R P$;
  output probability P at time t;
  $t = t + \tau_Q$;
end while

between stable states. It has been observed in many systems. Stochastic resonance has been observed in climate system, electronic circuits, neuron neuron systems, and others. In addition, it was applied to detect faults in rotational machinery [31] and optimize the potential well for energy harvesting [32, 33].

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

$$\frac{\partial}{\partial t}p(x_1,x_2,t) = -\frac{\partial}{\partial x_1}(g_1(x_1,x_2)p(x_1,x_2,t)) - \frac{\partial}{\partial x_2}(g_2(x_1,x_2)p(x_1,x_2,t)) + D\frac{\partial^2}{\partial x_2^2}p(x_1,x_2,t) \quad (24)$$

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

$$g_1(x_1,x_2) = x_2$$
$$g_2(x_1,x_2,t) = x_1 - 2\zeta\varepsilon x_2 - a_0\sin(2\pi f_0 t)$$

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

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

In this example, the values of the parameters are $\zeta = 0.5$, $\varepsilon = 1.0$, $D = 1.0$, $a_0 = 20$, 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 operator is developed to simulate stochastic diffusion processes in two- or higher-dimensional spaces. The operator enables the accelerated simulation of diffusion processes as quantum walks on graphs or dynamic real-time quantum systems. The continuous-time quantum walk is combined with random walks in imaginary-time systems or path integral. The proposed mathematical formalism is a generalization of the previous formulation for one-dimensional systems and supports various stochstic diffusion processes. The advantages of the proposed approach is the significant acceleration of simulation with much larger time step sizes than the ones used in path integral. The acceleration is particularly helpful for nonlinear system dynamics such as stochastic resonance, where the systems oscillates between stable states. The quantum tunneling effect helps the acceleration while avoiding the issue of possibly missing stable states in traditional path integral.

Similar to path integral, the proposed formulation is still based on Gaussian type of noises. Gaussian distribution is assumed in the short-time transition probabilities in the path integral formulation. As a result, the time step has to be small enough. Quantum walks with non-Gaussian distributions in the proposed formalism require investigation. The space complexity of the new formalism is the same as the one in path integral. Therefore, the computational efficiency is still limited by the state space if very high fidelity solutions are needed. In addition, it was assumed that the diffusion on graphs is homogeneously dependent on the topological distances. The anisotropicity of diffusion thus needs to be modeled. Geometry and orientation information thus needs to be included in future extension.

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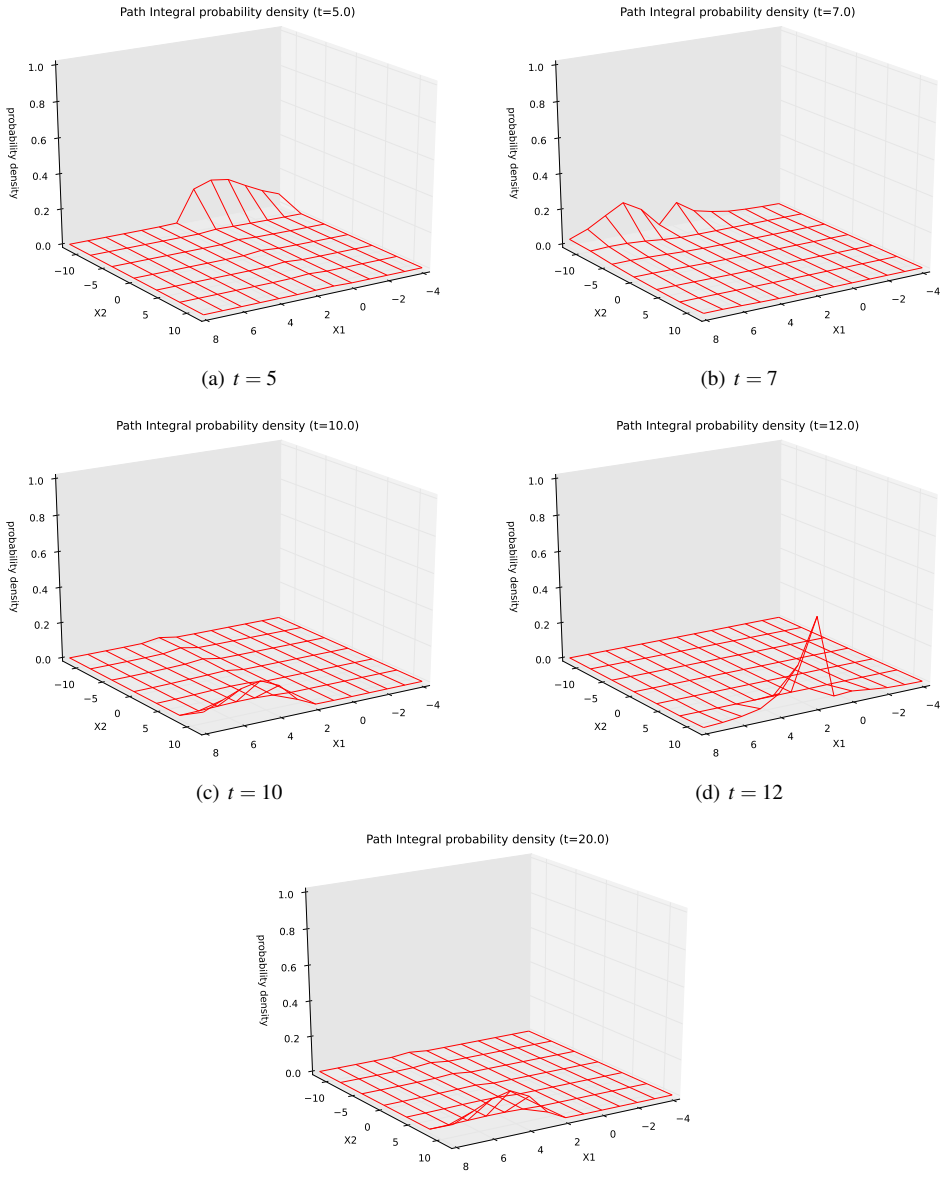

(a) $t = 5$

(b) $t = 7$

(c) $t = 10$

(d) $t = 12$

(e) $t = 20$

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

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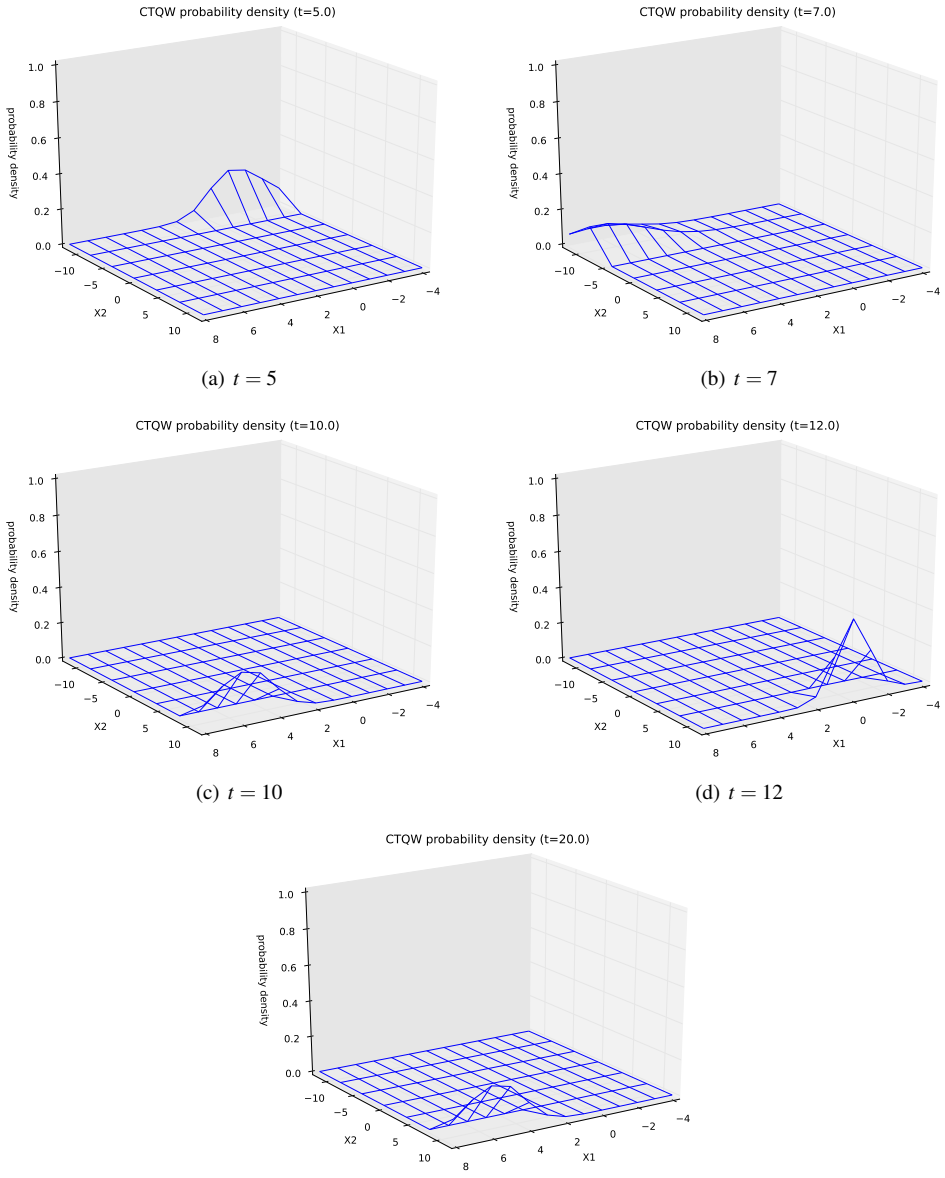

(a) $t = 5$ (b) $t = 7$

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

(e) $t = 20$

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

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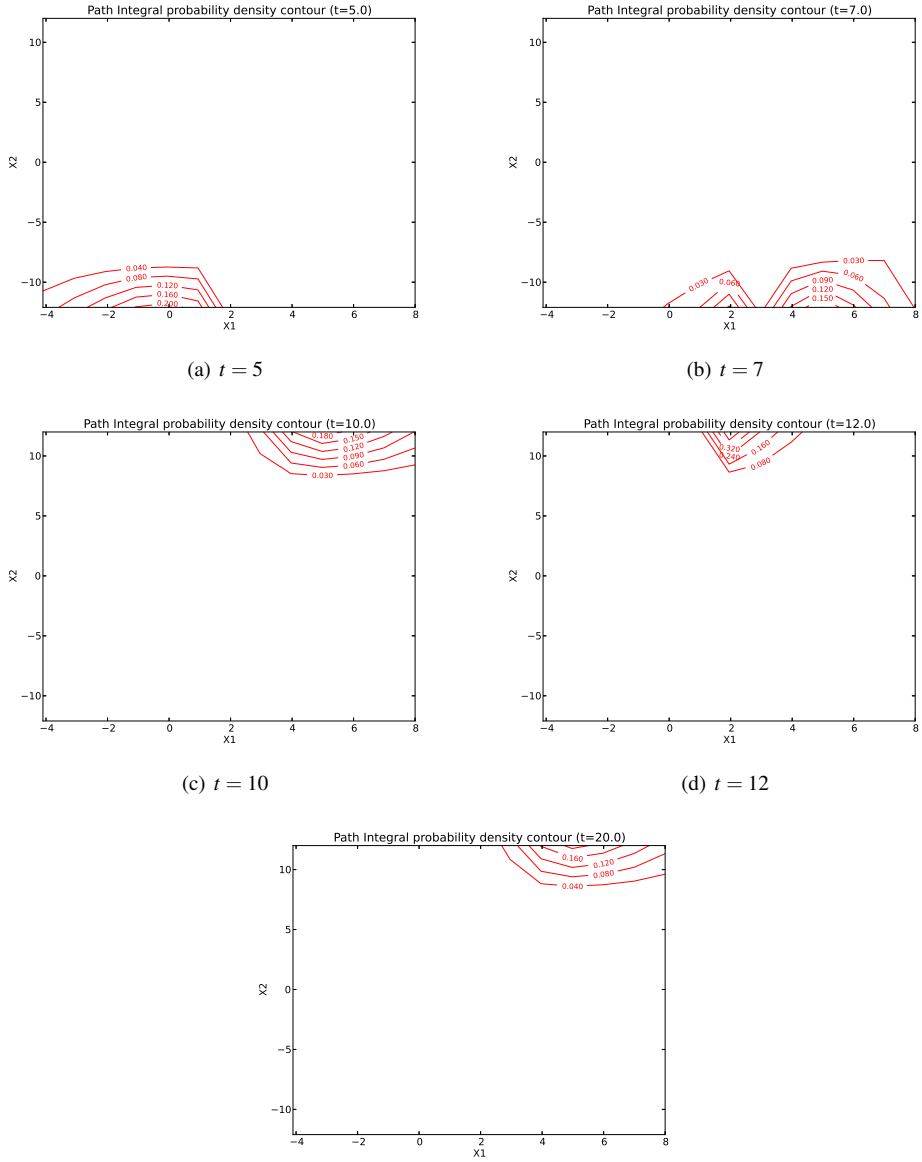

(a) $t = 5$

(b) $t = 7$

(c) $t = 10$

(d) $t = 12$

(e) $t = 20$

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

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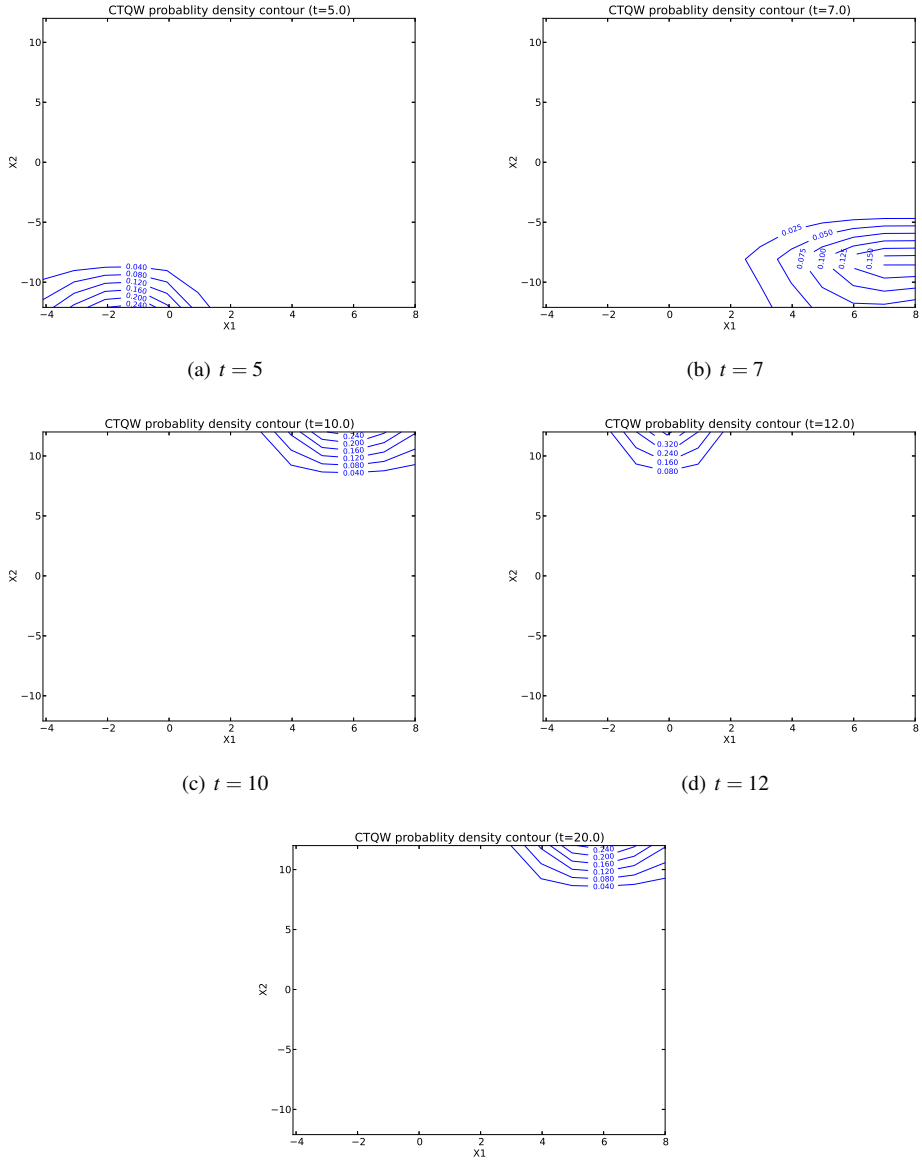

(a) $t = 5$

(b) $t = 7$

(c) $t = 10$

(d) $t = 12$

(e) $t = 20$

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

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