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Simulation of drift-diffusion processes by quantum walks

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ABSTRACT: Different from the Monte Carlo sampling approach to solve stochastic differential equations, the Fokker-Planck equation (FPE) models the dynamics of the probability density for all possible states. The evolution of the distribution is solved by the path integral alike methods. The major challenges of solving FPEs include the memory requirement to store transition matrix in a fine-grained state space and the small time step required for accurate estimation of short-time transition probabilities. In this paper, a new approach is presented to accelerate the simulation of stochastic dynamics under a new computational paradigm, quantum computing. A generic continuous-time quantum walk formulation is proposed to model stochastic drift-diffusion processes. With a second formulation that combines quantum and random diffusions, drastic acceleration can be achieved by taking advantages of non-local correlation in quantum systems, compared to the traditional path integral method.

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

In this paper, a new approach to accelerate computation in simulating stochastic dynamics is proposed, which is under an emerging computational paradigm, quantum computing. Quantum computer takes advantage of quantum mechanical systems to solve complex problems that require much more memory space and time in the classical computer. The basic computation unit is called qubit, which is mathematically regarded as a vector in a two-dimensional (2-D) complex vector space with inner product (i.e. Hilbert space). An N-qubit system can represent the state space of 2^N dimensions efficiently, where the associated complex-valued coefficients or amplitudes under the normalization condition correspond to the probabilities that the system is at a particular state.

Here a generic quantum mechanical formulation is developed to model stochastic drift-diffusion processes. It is based on continuous-time quantum walks. By solving an imaginary-time quantum system, the evolution of probability distributions in random diffusions can be captured. The numerical results show that the proposed formulation provides an effective approach to simulate stochastic drift-diffusion processes. More importantly, with a second formulation that combines quantum and random diffusions, drastic acceleration can be achieved by the use of non-local correlation in quantum systems. 1-D numerical examples show that the simulation can be hundreds of times faster than the traditional path integral method.

In the remainder of the paper, Section 2 provides the background of numerical methods of solving FPEs and

quantum walks. Section 3 presents the quantum walk formulation of random diffusion processes. Section 4 describes the quantum walk formulation of quantum diffusion and the combined algorithm to accelerate the stochastic drift-diffusion processes. Section 5 gives numerical examples to demonstrate the effectiveness and efficiency of the proposed approach.

2 BACKGROUND

2.1 *Solving fokker-planck equations for stochastic diffusions*

Various numerical methods to solve FPEs have been developed, including Monte Carlo (Ermak & Buckholz 1980), finite element (Masud & Bergman 2005), finite difference (Park & Petrosian 1996), spectral approximation (Wei 1999, Spanos, Sofi, & Di Paola 2007), and path integral (Haken 1975).

In particular, the path integral method has been shown as a simple yet accurate approach. It typically uses a short-time transition probability density matrix to approximate the evolution of drift-diffusion processes (Wehner & Wolfer 1983). Numerical efficiency and accuracy can be improved by interpolation of continuous density functions with discrete states (Naess & Johnsen 1993, Spencer & Bergman 1993, Naess & Moe 2000, Narayanan & Kumar 2012). Efficiency can be further improved in special problems (Kougioumtzoglou & Spanos 2012) or with special forms of distributions (Di Paola & Santoro 2008).

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 (Meyer 1996, Ambainis, Bach, Nayak, Vishwanath, & Watrous 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 & 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 convergence of discrete-time quantum walks toward continuous-time quantum walks has been demonstrated (Strauch 2006, Childs 2010).

3 QUANTUM WALK FORMULATION OF STOCHASTIC DIFFUSION

In this paper, the dynamics of probability distribution in drift-diffusion processes is formulated as continuous-time quantum walks. In the new formulation, a stochastic drift-diffusion process is modeled as an imaginary-time quantum system, described by

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

where $\hat{H}(t)$ is a generic Hamiltonian, and $\psi(x, t)$ is the *probability amplitude* for the system that is found to be at state x at time t. A transition rate from state x_k to state x_j is defined as

$$\rho_{jk}e^{i\theta_{jk}} := -\langle x_j|\hat{H}|x_k\rangle \tag{2}$$

where $i = \sqrt{-1}$, ρ_{jk} ($\rho_{jk} \geq 0$) is the magnitude of transition, and θ_{jk} is the phase shift associated with the transition. Then the probability magnitude of leaving state x_k is

$$\rho_k := \sum_{k\neq j} \rho_{jk} \tag{3}$$

and the overall transition rate for state x_k is determined by

$$W_k := -\langle x_k|\hat{H}|x_k\rangle + \rho_k \tag{4}$$

A *path* $x(t)$ is defined as a function of time t. For instance, $x(t_0) = i$ and $x(t_0+\tau) = j$ represent the transitional path from state x_i to state x_j during a time period of τ. A general *functional integral* for the transition from state x_i to state x_j is given by (Farhi & Gutmann 1992)

$$F_{ji} := \int dq_{ji} e^{-i\int_{t_0}^{t_0+\tau} W_{x(s)}ds} \prod_{l\to k} e^{i\theta_{kl}} \tag{5}$$

where dq_{ji} is the probabilistic measure on the path from x_i to x_j, $\int_{t_0}^{t_0+\tau} W_{x(s)}ds$ gives the overall probability of all possible paths from x_i at time t_0 to x_j at time $t_0+\tau$. At time s, $W_{x(s)}$ takes the value given by Eq.(4). $e^{-i\int_{t_0}^{t_0+\tau} W_{x(s)}ds}$ can be regarded as the *weight* of transition from x_i to x_j. $\prod_{l\to k} e^{i\theta_{kl}}$ is the *total phase*

shift factor for all jumps in transition from x_i to x_j, where each of $e^{i\theta_{kl}}$ corresponds to the phase shift for one of the jumps during the transition.

With the functional integral in Eq.(5), the evolution of probability amplitude is computed by

$$\psi_j(t+\tau) = \frac{1}{N_0(t+\tau)} \sum_i F_{ji}\psi_i(t) \tag{6}$$

where $\psi_i(t)$ is the amplitude of state x_i at time t and $N_0(t+\tau)$ is the normalization factor.

3.1 *Random diffusion process*

The random diffusion process is described by

$$-\frac{\partial}{\partial t}\psi(x,t) = -\frac{b}{2}\frac{\partial^2}{\partial x^2}\psi(x,t) \tag{7}$$

where b is the diffusion coefficient. Consider a discretized 1-D lattice space that has a spacing Δ, where the states are simply denoted by integers as $x = \ldots, -2, -1, 0, 1, 2, \ldots$. Based on the finite difference approximation, the elements of the Hamiltonian matrix are given by

$$\langle j|\hat{H}|k\rangle = -\frac{b}{2\Delta^2}[\delta_{j,k-1} - 2\delta_{j,k} + \delta_{j,k+1}] \tag{8}$$

where $\delta_{j,k}$ is the Dirac delta function defined as $\delta_{j,k} = 0$ if $j \neq k$ and $\delta_{k,k} = 1$. That is, $\langle k-1|\hat{H}|k\rangle = -b/(2\Delta^2)$ for left jump, $\langle k+1|\hat{H}|k\rangle = -b/(2\Delta^2)$ for right jump, and $\langle k|\hat{H}|k\rangle = b/\Delta^2$. As a result of Eq.(2), for any transition with $k \neq j$, $\rho_{jk} = [\delta_{j,k-1} + \delta_{j,k+1}]b/(2\Delta^2)$, and $e^{i\theta_{jk}} = 1$. From Eq.(3), we have $\rho_k = \rho_{k-1,k} + \rho_{k+1,k} = b/\Delta^2$. From Eq.(4), we have $W_k = -b/\Delta^2 + b/\Delta^2 = 0$.

Consider that the 1-D transitions are memoryless and the transition rate is $b/(2\Delta^2)$ per unit time. The numbers of transitions to the left or right direction within a time period follows a Poisson distribution. That is, the probability that there are l transitions 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 transitions 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 in Eq.(5) for one path from state 0 to $n\Delta$ that has l left jumps is

$$dq_{n,0}^{(l)} = \frac{e^{-b\tau/2\Delta^2}(\frac{b\tau}{2\Delta^2})^l}{l!} \frac{e^{-b\tau/(2\Delta^2)}(\frac{b\tau}{2\Delta^2})^{n+l}}{(n+l)!} \tag{9}$$

With zero weight and no phase shift, the complete functional integral in Eq.(5) for random diffusion processes is the summation of Eq.(9) over all possible paths with $l = 0, \ldots, \infty$ as

$$\begin{aligned} F_{n,0} &= \sum_{l=0}^{\infty} dq_{ji}^{(l)} = e^{-b\tau/\Delta^2} \sum_{l=0}^{\infty} \frac{(\frac{b\tau}{2\Delta^2})^{2l+n}}{l!(n+l)!} \\ &= e^{-b\tau/\Delta^2} I_n(\frac{b\tau}{\Delta^2}) \end{aligned} \tag{10}$$

where $I_n(y)$ is the *modified Bessel function of first kind* with integer order n and input y ($y \geq 0$). Additionally, $I_{-n}(y) = I_n(y)$.

3.2 *Random drift-diffusion process*

The random drift-diffusion process is described by

$$-\frac{\partial}{\partial t}\psi(x,t) = -\frac{b}{2}\frac{\partial^2}{\partial x^2}\psi(x,t) - iV(x,t)\psi(x,t) \tag{11}$$

where $V(x,t)$ is the potential function. The elements of the Hamiltonian matrix are given by

$$\langle j|\hat{H}|k\rangle = -\frac{b}{2\Delta^2}\delta_{j,k-1} + (\frac{b}{\Delta^2} - iV_k)\delta_{j,k} - \frac{b}{2\Delta^2}\delta_{j,k+1} \tag{12}$$

Similar to Section 3.1, we have $\rho_{jk} = \frac{b}{2\Delta^2}[\delta_{j,k-1} + \delta_{j,k+1}]$ for $(k \neq j)$, $e^{i\theta_{jk}} = 1$, $\rho_k = b/\Delta^2$, and $W_k = -iV_k$.

Here, the weight in Eq.(5) 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.(9), the final functional integral for random drift-diffusion processes is

$$F_{n,0} = \sum_{l=0}^{\infty} e^{-b\tau V_n} dq_{ji}^{(l)} = e^{-(V_n + b/\Delta^2)\tau} I_n(\frac{b\tau}{\Delta^2}) \tag{13}$$

where V_n is the potential corresponding to the final state at time $t_0 + \tau$.

3.3 *Correspondence to FPEs and SDEs*

For 1-D state space where $x \in \mathbb{R}$, the FPE is

$$\frac{\partial}{\partial t}p(x,t) = -\frac{\partial}{\partial x}[a(x,t)p(x,t)] + \frac{1}{2}\frac{\partial^2}{\partial x^2}[b(x,t)p(x,t)]$$

where $a(x,t)$ and $b(x,t)$ ($b \geq 0$) are the drift and diffusion coefficients respectively. The equivalent quantum

walk based drift-diffusion equation, as a generalization of Eq.(11), is

$$\frac{\partial}{\partial t}\psi(x,t) = \frac{1}{2}\frac{\partial^2}{\partial x^2}[b(x,t)\psi(x,t)] + iV(x,t)\psi(x,t)$$

where $\psi^*\psi = p$, and the potential V is related to the drift coefficient a as $\partial V(x,t)/\partial t = -a(x,t)$ or $V(x,t) = -a(x,t)x + A_0$ where A_0 is a constant that represents a potential shift. Notice that the value of A_0 is not important because the normalization procedure in Eq.(6).

The corresponding SDE is

$$dx = a(x,t)dt + b(x,t)d\mathcal{W}(t)$$

where $\mathcal{W}(t)$ denotes the Wiener process.

The algorithm to simulate stochastic drift-diffusion processes by quantum walks is listed in Table 1. Compared to the traditional path integral method, this algorithm takes the advantage of the extra information about the long range correlation between states in the form of Bessel functions. In the traditional path integral method, such information is not available. Therefore, the short-time transition probability is restricted to small τ. In contrast, the numerical efficiency can be improved based on the proposed quantum walk formulation with longer time steps. The examples in Section 5 will demonstrate that the time step can be 5 to 10 times longer than the one in the traditional path integral. Yet, the most significant improvement on time step efficiency by the proposed quantum walk approach comes from a second quantum walk formulation that simulates quantum diffusion, which will be described next in Section 4. The examples in Section 5 will show that the second algorithm with the combination of quantum and random diffusions can make the time step increment hundreds of times larger.

Table 1. The quantum walk algorithm to simulate stochastic diffusion processes based on the formulation of random diffusion.

Random_Drift_Diffusion()
Input: initial state $\psi_0(x)$, diffusion coefficient $b(t)$, potential function $V(x,t)$, time step τ, simulation time T
Output: final state $\psi(x)$

$\psi = \psi_0(x)$;
$t = 0$;
WHILE $t < T$
    update unitary operator $U = F(\tau, b, V, x, t)$ by Eq.(13);
    $|\psi\rangle = U|\psi\rangle$;
    $t = t + \tau$;
END

4 QUANTUM WALK FORMULATION OF QUANTUM DIFFUSION

The Schrödinger equation

$$i\frac{d}{dt}\psi(\mathbf{x},t) = \hat{H}(t)\psi(\mathbf{x},t) \tag{14}$$

describes quantum diffusion, where $\hat{H}(t)$ is the Hamiltonian. The transition rate from state x_k to state x_j is $\rho_{jk}e^{i\theta_{jk}} := -i\langle x_j|\hat{H}|x_k\rangle$. Notice the extra phase shift of i for a transition. Similarly, the probability magnitude of leaving state x_k is $\rho_k := \sum_{k\neq j}\rho_{jk}$ and the overall transition rate for state x_k is determined by $W_k := \langle x_k|\hat{H}|x_k\rangle + i\rho_k$.

Similar to Section 3, continuous-time quantum walks can be formulated to model the quantum diffusion and drift-diffusion processes.

4.1 *Quantum diffusion process*

The quantum diffusion process is described by

$$i\frac{\partial}{\partial t}\psi(x,t) = -\frac{b}{2}\frac{\partial^2}{\partial x^2}\psi(x,t) \tag{15}$$

where b is the diffusion coefficient. The elements of the Hamiltonian matrix for 1-D lattice space are the same as Eq.(8). For any transition with $k \neq j$, $\rho_{jk} = \frac{b}{2\Delta^2}[\delta_{j,k-1} + \delta_{j,k+1}]$, $e^{i\theta_{jk}} = i$, $\rho_k = \rho_{k-1,k} + \rho_{k+1,k} = \frac{b}{\Delta^2}$, and $W_k = \frac{b}{\Delta^2} + i\frac{b}{\Delta^2}$.

The probabilistic measure in Eq.(9) still applies. The weight in Eq.(5) now is $e^{-i\int_{t_0}^{t_0+\tau} W_{x(s)}ds} = e^{-i\tau(1+i)b/\Delta^2}$. For each small jump to the left or right, there is a phase shift of i. Therefore there is a total phase shift of $i^l i^{n+l} = i^{2l+n} = (-1)^l i^n$ for l left jumps and $n+l$ right jumps. Then the complete functional integral for quantum diffusion processes becomes

$$\begin{aligned} F_{n,0} &= \sum_{l=0}^{\infty}[dq_{ji}^{(l)}e^{-i\tau(1+i)b/\Delta^2}(-1)^l i^n] \\ &= i^n e^{-ib\tau/\Delta^2}\sum_{l=0}^{\infty}\frac{(-1)^l(\frac{b\tau}{2\Delta^2})^{2l+n}}{l!(n+l)!} \\ &= i^n e^{-ib\tau/\Delta^2}J_n(\frac{b\tau}{\Delta^2}) \end{aligned} \tag{16}$$

where $J_n(y)$ is the *Bessel function of first kind* with integer order n and input y ($y \geq 0$). Additionally, $J_{-n}(y) = (-1)^n J_n(y)$.

4.2 *Quantum drift-diffusion process*

The quantum drift-diffusion process is described by

$$i\frac{\partial}{\partial t}\psi(x,t) = -\frac{b}{2}\frac{\partial^2}{\partial x^2}\psi(x,t) - iV(x,t)\psi(x,t) \tag{17}$$

where b is the diffusion coefficient and V is the potential function. The elements of the Hamiltonian matrix for 1-D lattice space are the same as Eq.(12). For any transition with $k \neq j$, $\rho_{jk} = \frac{b}{2\Delta^2}[\delta_{j,k-1} + \delta_{j,k+1}]$, $e^{i\theta_{jk}} = i$, $\rho_k = \rho_{k-1,k} + \rho_{k+1,k} = \frac{b}{\Delta^2}$, and $W_k = \frac{b}{\Delta^2} - iV_k + i\frac{b}{\Delta^2}$.

For a transition with n steps away from the initial state for a total period τ, the weight in the functional integral 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.(9) and similar to the derivation of Eq.(16), the complete functional integral for quantum drift-diffusion processes is

$$F_{n,0} = i^n e^{-ib\tau/\Delta^2 - V_n\tau} J_n(\frac{b\tau}{\Delta^2}) \tag{18}$$

4.3 *Quantum acceleration*

The wave of quantum diffusion propagates quadratically faster than the random diffusion. By taking advantage of the strong non-local correlation in quantum diffusion, we combine the quantum walk for quantum diffusion with the one for random diffusion, which significantly accelerates the simulation of stochastic diffusion.

Table 2 lists the new algorithm with the combination of quantum walks for quantum diffusion and random diffusion. Two different time steps, τ_Q for quantum diffusion and τ_R for random diffusion, are needed. The timing of simulation is based on τ_Q, since the two respective systems for quantum and random diffusions are in two orthogonal time domains. A large τ_Q can be chosen so that the acceleration is achieved.

Table 2. The quantum walk algorithm to simulate stochastic diffusion processes based on the formulation of quantum and random diffusions.

Quantum_Random_Drift_Diffusion()
Input: initial state $\psi_0(x)$, diffusion coefficient $b(t)$, potential function $V(x,t)$, time step τ_Q, time step τ_R, simulation time T
Output: final state $\psi(x)$

$\psi' = \psi_0(x)$;
$t = 0$;
WHILE $t < T$
    update operator $U_Q = F(\tau_Q, b, V, x, t)$ by Eq.(18);
    $|\psi'\rangle = U_Q|\psi'\rangle$;
    update operator $U_R = F(\tau_R, b, V, x, t)$ by Eq.(13);
    $|\psi\rangle = U_R|\psi'\rangle$;
    $t = t + \tau_Q$;
END

5 NUMERICAL EXAMPLES

We developed a quantum computing emulator and the 1-D quantum walk formulation was implemented and tested in this environment. Here two examples are used to demonstrate. The first example is a diffusion process with a linear drift and the second one is a bi-stable stochastic resonance system. The effectiveness of the proposed approach is first demonstrated by comparisons with the traditional FPE path integral and SDE Monte Carlo sampling methods. Then the efficiency of the new approach compared to the path integral method is demonstrated.

5.1 *Linear drift diffusion process*

The SDE for the diffusion process with a linear drift coefficient is

$$dx = (c_1 x + c_2)dt + \sigma d\mathcal{W}$$

The corresponding potential function in the quantum walk formulation is

$$V(x) = -c_1 x^2 - c_2 x$$

The first set of parameters used in this example are $c_1 = -0.1$, $c_2 = 0.2$, and $\sigma = 0.3$. With the initial distribution $p(x = 5.0) = 1.0$, the results calculated by the proposed quantum walk formulation and the traditional path integral method based on FPEs are shown in Figure 1. The time steps used for the two methods are both $\tau = 0.2$.

A further comparison among the quantum walk formulation, path integral, and Monte Carlo (MC) sampling based on SDEs are shown in Figure 2 where the distributions at times $t = 6$ and $t = 70$ are compared. The number of sample trajectories used in the SDE sampling is 50,000. The second set of parameters used are $c_1 = -0.1$, $c_2 = 0.2$, and $\sigma = 0.6$. With the same initial distribution and time step, the results of the three methods are compared in Figure 3. With a

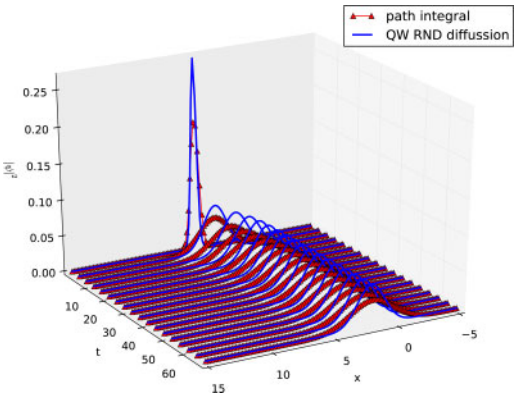


Figure 1. Comparison between the results of the quantum walk and FPE path integral methods for the linear drift diffusion $\sigma = 0.3$.

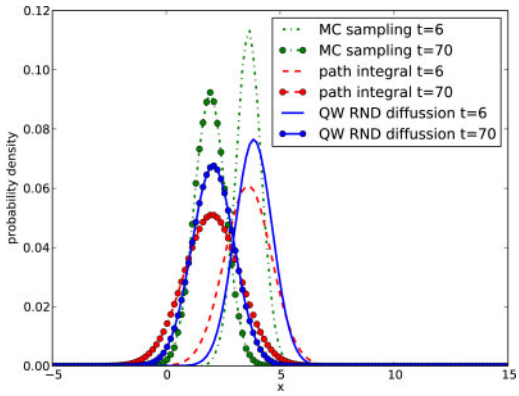


Figure 2. Comparison of distributions from the quantum walk, FPE path integral, and SDE MC sampling methods for the linear drift diffusion $\sigma = 0.3$.

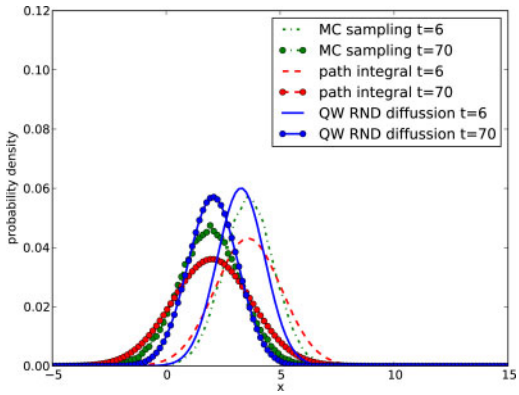


Figure 3. Comparison of distributions from the quantum walk, FPE path integral, and SDE MC sampling methods for the linear drift diffusion $\sigma = 0.6$.

larger diffusion coefficient than the previous one, the distribution spreads wider. It is seen that the quantum walk formulation gives the similar results as the path integral and the SDE sampling methods.

5.2 *Bi-stable stochastic resonance*

The bi-stable stochastic resonance phenomenon is a nonlinear response of a system with sinusoidal inputs simultaneously subject to noises, where the system oscillates between two states as transitions. The example system is modeled by the SDE

$$\frac{dx}{dt} = c_1 x - c_2 x^3 + a_0 \sin(2\pi f_0 t) + N(t)$$

where state x changes along time t, c_1 and c_2 are coefficients, a_0 and f_0 are the amplitude and modulation frequency of the periodic input respectively, and the noise $N(t) = \sqrt{2B}\xi(t)$ has the intensity of B with $\mathbb{E}[N(t), N(t+s)] = 2B\delta(s)$, $\delta(\cdot)$ is the Dirac delta function, and $\xi(t)$ is a zero-mean, unit variance

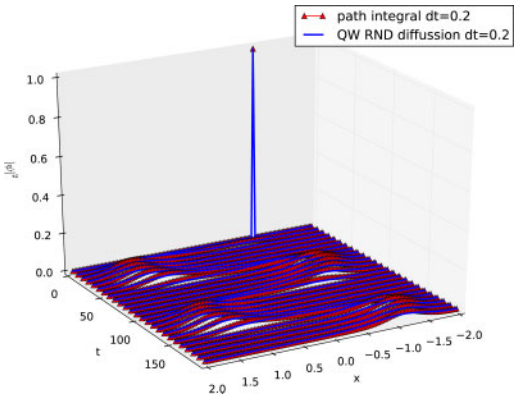


Figure 4. Comparison between the results of the quantum walk and FPE path integral methods.

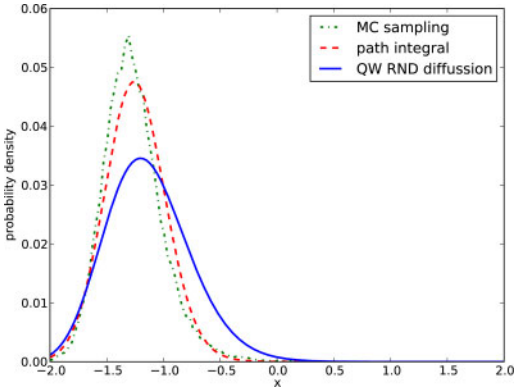


Figure 5. comparison of distributions from the quantum walk, FPE path integral, and SDE MC sampling methods at time $t = 80$.

Gaussian white noise. The drift and diffusion coefficients of the corresponding FPE are

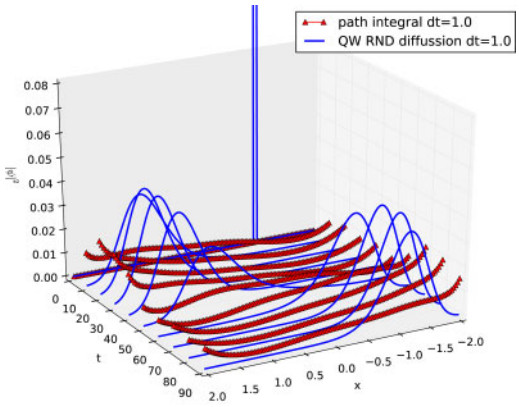
$$A(x,t) = c_1 x - c_2 x^3 + a_0 \sin(2\pi f_0 t)$$

and B respectively. In the quantum walk formulation of Eq.(11), the potential function used here is

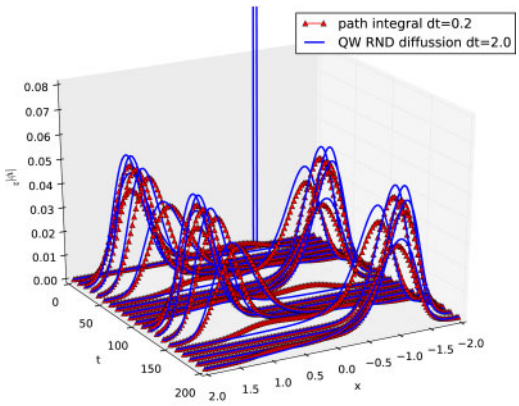
$$V(x,t) = -c_1 x^2/2 + c_2 x^4/4 - a_0 \sin(2\pi f_0 t) x$$

In this example, the parameter values are $c_1 = 1$, $c_2 = 1$, $a_0 = 1$, $f_0 = 0.01$, and $B = 0.31$. The range of x in the state space is between -2 and 2. The chosen time step size is $\tau = 0.2$. The initial distribution is chosen as $p(x = -1.0) = 1.0$. Figure 4 shows the comparison between the new quantum walk formulation and the traditional path integral method for the same problem. Different from the previous example, it is seen that the variation range predicted by the quantum walk method is slightly larger than that of the traditional path integral method by a closer look.

A further comparison is done with the MC trajectories to solve the corresponding SDE. Figure 5 shows



(a) $\tau = 1.0$

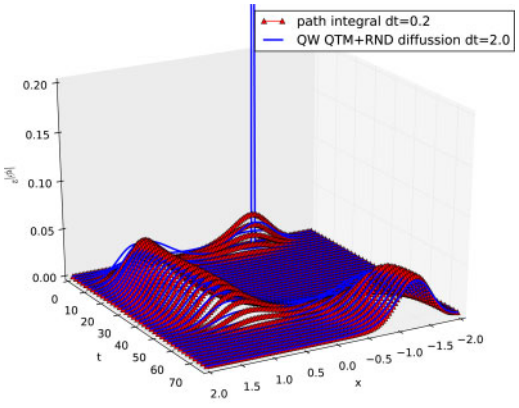


(b) $\tau = 2.0$

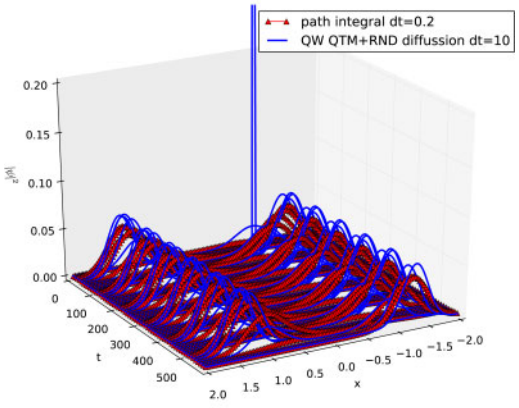
Figure 6. Comparison between the quantum walk and FPE path integral methods with different time step τ.

the typical results from the three methods, which are at time $t = 80$, where $50,000$ trajectories are sampled in the MC simulation. Again, it is seen that the new quantum walk formulation has the similar accuracy as the path integral method.

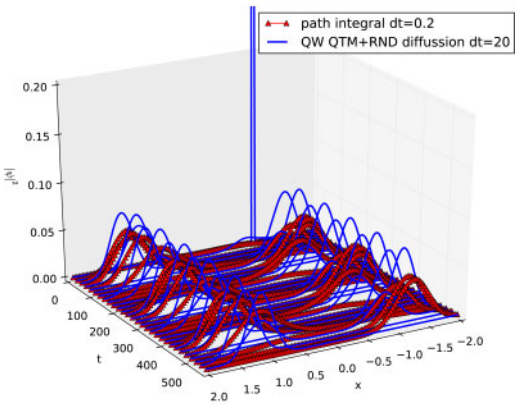
The simulation acceleration of the quantum walk formulation is also demonstrated by the bi-stable stochastic resonance system. When time step size τ increases, the distributions calculated by the tradition path integral method tend to spread out. When the time step reaches $\tau = 0.6$, the distributions can become very different from the original solution. Figure 6 compares the results of the quantum walk based on random diffusion only and FPE path integral methods with different time step sizes. The bistable resonance phenomenon has disappeared in the path integral simulation, as shown in Figure 6-(a). In contrast, there is little change in the simulation by quantum walks. Even when a large step size of $\tau = 2.0$ is taken in quantum walk, as shown in Figure 6-(b), it is still similar to the original one from



(a) $\tau_Q = 2.0$



(b) $\tau_Q = 10$



(c) $\tau_Q = 20$

Figure 7. Drastic acceleration achieved by the combination of quantum and random diffusions.

the path integral method with the step size $\tau = 0.2$. To reach the time $t = 200$, it takes 1000 iterations with $\tau = 0.2$. However, the similar result is obtained by only 100 iterations with $\tau = 2.0$ by the quantum walk method.

The drastic acceleration is achieved by the combined quantum-random diffusion simulation described in Section 4.3. For each iteration of simulation, a very large step of quantum diffusion is followed by a small step of random diffusion. Figure 7 shows four different choices of quantum diffusion step size τ_Q. For each one of the four cases, the random diffusion step size is $\tau_R = 0.2$. It is seen that the choices of large step sizes can accelerate the simulation significantly. For the case of $\tau_Q = 20$, the simulation is 100 times faster than the path integral with $\tau = 0.2$.

6 CONCLUSIONS

In this paper, the potential of quantum computation in stochastic simulation has been demonstrated. A new continuous-time quantum walk formulation is developed to simulate stochastic diffusion processes. The random drift-diffusion process is modeled as the dynamics of imaginary-time quantum systems. The formulation is generic and applicable to diffusions with specific potential functions available.

In the traditional path integral method, the assumption of Markovian property results in the independence between states that are not immediately adjacent. Thus the long-range interaction is not modeled. In contrast, quantum walks can represent the spatial correlation or coherence with longer distances as quantum dynamics by the Bessel functions. By combining quantum and random diffusions in a quantum system, the quantum effect of non-local correlation can have a quadratic speed-up compared to classical random walks. This acceleration has significantly improved the efficiency of diffusion process simulation.

The test examples have showed the effectiveness of the new approach in comparison with the traditional path integral and Monte Carlo sampling. More rigorous error study is needed in the future to compare the accuracies among the three approaches. The current implementation of the new algorithms is still on classical computers, which has not fully harnessed the power of quantum computers yet. The mechanisms of superposition and quantum parallelism of a quantum computer will dramatically accelerate stochastic simulation with much greater accuracy.

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