The Annals of Applied Statistics
2011, Vol. 5, No. 2A, 669–683
DOI: 10.1214/10-AOAS406

QUANTUM MONTE CARLO SIMULATION[1]

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Contemporary scientific studies often rely on the understanding of complex quantum systems via computer simulation. This paper initiates the statistical study of quantum simulation and proposes a Monte Carlo method for estimating analytically intractable quantities. We derive the bias and variance for the proposed Monte Carlo quantum simulation estimator and establish the asymptotic theory for the estimator. The theory is used to design a computational scheme for minimizing the mean square error of the estimator.

1. Introduction. Computer-aided simulations of physical systems are widely used in scientific and engineering studies such as aircraft and car design and nuclear explosion modeling. While the traditional simulation methods with the aid of classical computers based on transistors are to understand basic properties of materials, many contemporary simulations rely on understanding quantum systems, such as those in bio-chemistry and nano-technology for the design of nano-materials and novel molecules. See Aspuru-Guzik et al. (2005), Kou (2009) and Waldner (2007).

A quantum system is described by its state, which is often characterized by a vector in some complex Hilbert space. The number of complex numbers required to characterize the quantum state normally grows exponentially with the size of the system, rather than linearly, as occurs in classical physical systems. Consequently, for a quantum system it takes an exponential number of bits of memory on a classical computer to store its quantum state, and simulations of quantum systems via classic computers face great computational challenge. As quantum systems are able to store and keep track an exponential number of complex numbers and perform data manipulations and calculations as the systems evolve, quantum computation and quantum information are to grapple with understanding how to take advantage of the enormous information hidden in quantum systems and to harness the immense potential computational power of atoms and molecules for the purpose of information processing and computation. Quantum computers built upon quantum systems may excel in the simulation of naturally occurring quantum systems, where such quantum systems may be hard to simulate in an efficient

Received January 2010; revised August 2010.
[1]Supported in part by the NSF Grant DMS-10-05635.
Key words and phrases. Asymptotic theory, estimation, Monte Carlo, qubit, quantum computation, quantum statistics.

manner by classical computers [Abrams and Lloyd (1997), Boghosian and Taylor (1998) and Zalka (1998)].

To the best of our knowledge, this paper is the first to introduce quantum computation and study quantum simulation in the statistical framework. Specifically, we will propose a Monte Carlo quantum simulation method for computing analytically intractable quantities and analyze approximation errors and random variations of the proposed Monte Carlo estimator. The theoretical analysis establishes a strategy to design an optimal scheme for utilizing computational resources in obtaining the Monte Carlo estimator.

The rest of the paper proceeds as follows. Section 2 provides a brief review on quantum mechanics, quantum statistics and basic concepts of quantum computation. Section 3 proposes a Monte Carlo quantum simulation method and then presents the statistical analysis for the method. We derive the variance and bias for the proposed estimator and establish the strategy to allocate computational resources in the Monte Carlo quantum simulation for minimizing the mean square error of the estimator. A quantum simulation example is illustrated in Section 4.

2. Brief background review.

2.1. *Quantum physics*. Quantum mechanics describes phenomena at microscopic level such as position and momentum of an individual particle like an atom or electron, spin of an electron, detection of light photons, and the emission and absorption of light by atoms. Unlike classical mechanics where measurements of quantities like position and momentum can be observed accurately, the quantum theory can only make statistical prediction about the results of the measurements performed.

Mathematically quantum mechanics is usually described by a Hilbert space $\mathcal{H}$ and Hermitian (or self-adjoint) operators on $\mathcal{H}$. As in quantum mechanics, we adopt standard Dirac notation $|\cdot\rangle$, which is called a ket, to indicate that the object is an element in $\mathcal{H}$. A quantum system is completely described by its state and the time evolution of the state. A state is often classified as a pure state or an ensemble of pure states that are easy to describe by density operators. A pure state is a unit vector $|\psi\rangle$ in $\mathcal{H}$, which corresponds to a density operator $\rho = |\psi\rangle\langle\psi|$, the projection operator on $|\psi\rangle$. An ensemble of pure states corresponds to the case that the quantum system is in one of states $|\psi_k\rangle$, $k = 1, \ldots, K$, with probability p_k being in state $|\psi_k\rangle$, and the corresponding density operator is

$$\rho = \sum_{k=1}^{K} p_k |\psi_k\rangle\langle\psi_k|. \tag{1}$$

Let $|\psi(t)\rangle$ be the state of the quantum system at time t. The states $|\psi(t_1)\rangle$ and $|\psi(t_2)\rangle$ at t_1 and t_2 are connected through $|\psi(t_2)\rangle = U(t_1, t_2)|\psi(t_1)\rangle$, where

$U(t_1, t_2)$ is a unitary operator depending only on time t_1 and t_2. In fact, there exists a Hermitian operator H, which is known as the Hamiltonian of the quantum system, such that $U(t_1, t_2) = \exp[-iH(t_2 - t_1)]$. With Hamiltonian H, we may depict the continuous time evolution of $|\psi(t)\rangle$ by Schrödinger's equation

$$i\frac{\partial|\psi(t)\rangle}{\partial t} = H|\psi(t)\rangle. \tag{2}$$

See Holevo (1982) and Sakurai (1995).

2.2. *Quantum probability.* Quantum mechanics can be tested by checking its predications with experiments of performing measurements on quantum systems. The common quantum measurements are on observables such as position, momentum, spin and so on, where an *observable* is defined as a Hermitian operator on Hilbert space $\mathcal{H}$. Consider an observable $\mathbf{X}$ with a discrete spectrum so that it can be written in a diagonal form

$$\mathbf{X} = \sum_{a=1}^{p} x_a \mathbf{Q}_a, \tag{3}$$

where $x_a \in \mathbb{R}$ are eigenvalues of $\mathbf{X}$ and $\mathbf{Q}_a$ are the corresponding one-dimensional projections onto the eigenvectors of $\mathbf{X}$. Possible measurement outcomes of the observable are described by measure space $(\Omega, \mathcal{F})$. For a quantum system with state ρ, the result of the measurement is random with probability distribution P_ρ over $(\Omega, \mathcal{F})$. We denote by X the result of the measurement of observable $\mathbf{X}$ given by (3). The result X is a random variable and takes values in $\Omega = \{x_1, x_2, \ldots\}$. With a quantum system prepared in the state ρ, the result X has a probability distribution $P_\rho[X = x_a] = \operatorname{tr}(\rho \mathbf{Q}_a)$. With the probability distribution P_ρ, we can easily derive the expectation and variance of $\mathbf{X}$ in the state

$$E_\rho[\mathbf{X}] = \operatorname{tr}(\rho\mathbf{X}) = \sum_{a=1}^{p} x_a P_\rho[X = x_a] = E_{P_\rho}(X),$$

$$\operatorname{Var}_\rho[\mathbf{X}] = \operatorname{tr}[\rho\mathbf{X}^2] - [\operatorname{tr}(\rho\mathbf{X})]^2.$$

Measuring the outcomes of observable $\mathbf{X}$ will alter the state of the quantum system. If the state of the quantum system is ρ immediately before the measurement, then the probability that the result x_a occurs is $P_\rho[X = x_a] = \operatorname{tr}(\rho\mathbf{Q}_a)$ and the state of the system after the measurement result x_a is equal to $\mathbf{Q}_a\rho\mathbf{Q}_a / \operatorname{tr}(\mathbf{Q}_a\rho\mathbf{Q}_a)$. Similarly, using the spectral theory of self-adjoint operators, we may describe observables with continuous spectrum and continuous measurement outcomes. See Barndorff-Nielsen, Gill and Jupp (2003) and Holevo (1982).

2.3. *Quantum computation*. Quantum systems can be simulated via computers, but quantum simulation requires enormous computational resources. Classic computers may have great difficulty to efficiently simulate general quantum systems, while quantum computers built upon quantum systems are ideal for quantum simulation.

Analog to the fundamental concept of the bit in classical computation and classical information, we have quantum bit in quantum computation and quantum information and call it qubit for short. Just like a classical bit with state either 0 or 1, a qubit has states $|0\rangle$ and $|1\rangle$. However, there is a real difference between a bit and a qubit. Besides states $|0\rangle$ and $|1\rangle$, a qubit can also take states as their superpositions, which are the linear combinations of $|0\rangle$ and $|1\rangle$,

$$|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle,$$

where complex numbers α_0 and α_1 are called amplitudes satisfying $|\alpha_0|^2 + |\alpha_1|^2 = 1$. In other words, the states of a qubit are unit vectors in a two-dimensional complex vector space, and states $|0\rangle$ and $|1\rangle$ consist of an orthonormal basis for the space and are often referred to as computational basis states. The qubit is the simplest quantum system. Unlike a classical bit which can be examined to determine whether it is in the state 0 or 1, for a qubit we can not determine its state and find the values of α_0 and α_1 by examining it. Quantum mechanics shows that we can measure a qubit and obtain either the result 0, with probability $|\alpha_0|^2$, or the result 1, with probability $|\alpha_1|^2$. A qubit can be actually realized as physical objects in many different physical systems, such as the two different polarizations of a photon, the alignment of a nuclear spin in a uniform magnetic field or two states of an electron orbiting a single atom. In the atom model case, we may correspond $|0\rangle$ and $|1\rangle$ with the so-called "ground" or "excited" states of the electron, respectively. As the atom is shined by light with suitable energy and for a proper amount of time, we can move the electron from the $|0\rangle$ state to the $|1\rangle$ state and vice versa. Moreover, by shortening the length of time shining the light on the atom, we can move an electron initially in the state $|0\rangle$ to "halfway" between $|0\rangle$ and $|1\rangle$, say, into a state $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$.

Like classical bits, we may consider multiple qubits. The states of two qubits are unit vectors in a four-dimensional complex vector space, with four computational basis states labeled by $|00\rangle$, $|01\rangle$, $|10\rangle$ and $|11\rangle$. In general, a system of b qubits has 2^b computational basis states of the form $|x_1x_2\cdots x_b\rangle$, $x_j = 0$ or 1, $j = 1, \ldots, b$, that generate a 2^b-dimensional complex vector space, and a superposition state in the system is specified by 2^b amplitudes. As 2^b increases exponentially in b, it is easy for such a system to have an enormously big vector space. A quantum system consisting of even a few dozens of "qubits" will strain the resources of even the largest supercomputers. Consider a system with 50 qubits. $2^{50} \approx 10^{15}$ complex amplitudes are needed to depict its quantum state. With 128 bits of precision, it requires approximately 32 thousand terabytes of information to store all

10^{15} complex amplitudes. Had Moore's law continued on schedule, such storage capacity would be available in supercomputers during the second decade of the twenty-first century. A system with $b = 500$ qubits has the number of amplitudes larger than the estimated number of atoms in the universal. It is unimaginable to store all 2^{500} complex numbers in any classical computers. In principle, a quantum system with only a few hundred atoms can manage such an enormous amount of data and execute calculations as the system evolves. Quantum computation and quantum information are to find ways to utilize the immense potential computational power in quantum systems. See Clarke and Wilhelm (2008), Deutsch (1985), DiCarlo et al. (2009), Feynman (1982), Lloyd (1996), DiVincenzo (1995), Nielsen and Chuang (2000) and Shor (1994).

3. Statistical analysis of quantum simulation. The key for the simulation of a quantum system lies in the solution of Schrödinger's equation (2) which governs the dynamic evolution of the system, and the quantum simulation can be done via either classic computing or quantum computing. Schrödinger's equation for a typical Hamiltonian with real particles usually consists of elliptical differential equations, where each differential equation can be easily simulated by a classical computer. The real challenge in stimulating a quantum system is to solve the exponential number of such differential equations. Consider a quantum system that is described by b qubits. As b qubits have 2^b amplitudes, for stimulating the dynamic behavior of b qubits evolving according to Schrödinger's equation, a system of 2^b differential equations must be solved. Because of the exponential growth in the number of differential equations, simulating quantum systems by classical computers is feasible only for special cases where insightful approximations are available to dramatically reduce the effective number of differential equations involved. Quantum computers may be ideal for the simulation of naturally occurring quantum systems. See Abrams and Lloyd (1997), Boghosian and Taylor (1998), Feynman (1982), Lloyd (1996) and Zalka (1998). Whether quantum simulation is via classic computing or quantum computing, its statistical aspect essentially remains the same.

3.1. *Simulate a quantum system.* The heart of quantum simulation is to solve Schrödinger equation (2) which has the solution

$$|\psi(t)\rangle = e^{-iHt}|\psi(t_0)\rangle. \tag{4}$$

Numerical evaluation of e^{-iHt} is needed. The Hamiltonian H is usually exponentially large and extremely difficult to exponentiate. The common approach in numerical analysis that uses the first-order linear approximation, $1 - iH\delta$, of $e^{-iH(t+\delta)} - e^{-iHt}$ often yields unsatisfactory numerical solutions.

Efficient evaluation of the solutions (4) with high order approximation exists for many classes of Hamiltonians. For most physical systems the Hamiltonians involve only location interactions, which originate from the fact that most interactions fall

off with increasing distance or difference in energy. Specifically, a system of α particles in a d-dimensional space often has a Hamiltonian of the form

$$H = \sum_{\ell=1}^{L} H_\ell, \tag{5}$$

where L is a polynomial in $\alpha + d$, and each H_ℓ acts on a small subsystem of finite size free from α and d. Typical examples of the terms H_ℓ are one-body Hamiltonians and two-body interactions such as the ones in the Hubbard and Ising models [Altland and Simons (2006) and Dziarmaga (2005)]. As a result, $e^{-iH_\ell\delta}$ is easy to compute numerically, although $e^{-iH\delta}$ is very hard to evaluate. Because H_ℓ and H_k are noncommutable, $e^{-iH\delta} \neq e^{-iH_1\delta}\cdots e^{-iH_L\delta}$. Using the Trotter formula [Kato (1978), Sornborger and Stewart (1999) and Trotter (1959)], we approximate $e^{-iH\delta}$ by U_δ which requires only the evaluation of each $e^{-iH_\ell\delta}$, where

$$U_\delta = [e^{-iH_1\delta/2}\cdots e^{-iH_L\delta/2}][e^{-iH_L\delta/2}\cdots e^{-iH_1\delta/2}]. \tag{6}$$

Suppose that the quantum system starts at t_0 with initial state $|\psi(t_0)\rangle$ and ends at final time T. For an integer m, let $\delta = T/m$ and $t_j = j\delta$, $j = 0, 1, \ldots, m$. The quantum simulation is to apply approximation U_δ of $e^{-iH\delta}$ to solutions (4) at t_j iteratively and generate approximate solutions for $|\psi(t_j)\rangle$. Denote by $|\tilde{\psi}(t_j)\rangle$ the state at t_j obtained from the quantum simulation as an approximation of the true state $|\psi(t_j)\rangle$ at t_j. Then for $j = 1, \ldots, m$,

$$\begin{aligned} |\psi(t_j)\rangle &= e^{-iH\delta}|\psi(t_{j-1})\rangle = e^{-iHj\delta}|\psi(t_0)\rangle, \\ |\tilde{\psi}(t_j)\rangle &= U_\delta|\tilde{\psi}(t_{j-1})\rangle = U_\delta^j|\psi(t_0)\rangle. \end{aligned} \tag{7}$$

If the initial state of the quantum simulation is a pure state $|\psi(t_0)\rangle$, then the true final state and the simulated final state are also pure states $|\psi(t_m)\rangle$ and $|\tilde{\psi}(t_m)\rangle$, respectively, with corresponding density operators

$$\rho(t_0) = |\psi(t_m)\rangle\langle\psi(t_m)|, \qquad \tilde{\rho} = |\tilde{\psi}(t_m)\rangle\langle\tilde{\psi}(t_m)|.$$

When the initial state is an ensemble of pure states, with probability p_k being pure state $|\psi_k(t_0)\rangle$, $k = 1, \ldots, K$, and corresponding density operator

$$\rho(t_0) = \sum_{k=1}^{K} p_k|\psi_k(t_0)\rangle\langle\psi_k(t_0)|,$$

then at time t_j the true state and the simulated state are also ensembles of pure states with respective density operators

$$\rho(t_j) = \sum_{k=1}^{K} p_k|\psi_k(t_j)\rangle\langle\psi_k(t_j)|,$$

$$\tilde{\rho}(t_j) = \sum_{k=1}^{K} p_k|\tilde{\psi}_k(t_j)\rangle\langle\tilde{\psi}_k(t_j)|,$$

where for $k = 1, \ldots, K$,

$$|\psi_k(t_j)\rangle = e^{-iH\delta}|\psi_k(t_{j-1})\rangle = e^{-iHj\delta}|\psi_k(t_0)\rangle,$$
$$|\tilde{\psi}_k(t_j)\rangle = U_\delta|\tilde{\psi}_k(t_{j-1})\rangle = U_\delta^j|\psi_k(t_0)\rangle.$$

3.2. *Monte Carlo quantum simulation*. Quantum simulation provides an excellent way for the study of complex phenomena in physical and biology systems and evaluating hard-to-obtain quantities in the system. Examples include the dielectric constant, the mass of the proton, conductivity, magnetic susceptibility of materials and molecules in biological systems. As the results of quantum measurement outcome are random, repeated measurements need to be performed in order to obtain reliable estimators of the quantities. In the quantum setup, a quantity of interest is of the form

$$\theta = E_\rho(\mathbf{X}) = \mathrm{Tr}(\mathbf{X}\rho) = E_{P_\rho}(X), \tag{8}$$

where $\mathbf{X}$ is an observable, X is its measurement result, and ρ is the state of the quantum system under which we perform the measurements and evaluate the quantity θ.

A Monte Carlo quantum simulation method is designed to estimate θ as follows. We prepare the quantum system at initial state $\rho(t_0)$ and make it evolve to final state $\rho(t_m) = \rho$. The quantum simulation procedure described in Section 3.1 is used to simulate the evolutions of the quantum system from initial state $\rho(t_0)$ to final state $\rho(t_m)$ according to Schrödinger's equation (4) with some Hamiltonian H of the form given by (5). We repeatedly perform the measurements of observable $\mathbf{X}$ in such n identically simulated quantum systems at the simulated final state and obtain measurement results $X_1, \ldots, X_n$. We estimate θ defined in (8) by

$$\hat{\theta} = \frac{1}{n}\sum_{j=1}^{n} X_j. \tag{9}$$

Since measurements and state approximations in quantum simulation are involved with random fluctuations and systematic errors, $\hat{\theta}$ as a Monte Carlo estimator of θ has variance and bias. We use mean square error (MSE) criterion to gauge its performance. The Monte Carlo quantum simulation method for obtaining estimator $\hat{\theta}$ requires to repeat the simulation of the quantum system n times, and each simulation needs to calculate m approximations of states at t_j, $j = 1, \ldots, m$. The whole Monte Carlo quantum simulation procedure needs to make total $N = mn$ state approximations for the quantum system. One important problem is to determine the strategy to allocate m and n with given $N = mn$ so that the MSE of $\hat{\theta}$ is minimized. We derive the MSE of $\hat{\theta}$ and study the problem in the following theorem.

THEOREM 3.1. *For a quantum system evolving in time interval* $[0, T]$, *assume that its Hamiltonian* H *and observable* $\mathbf{X}$ *satisfy* (5) *in Section* 3.1 *and* (11) *in Section* 3.3, *respectively. Then*

$$E[(\hat{\theta} - \theta)^2] \le \frac{C_1}{n} + \frac{C_2}{m^4} = \frac{C_1}{N\delta} + \frac{C_2\delta^4}{T^4},$$

where C_1 *and* C_2 *are generic constants free from* m *and* n. *Thus, when* $n = C_1 m^4 / C_2$ *and* $m = (C_2/C_1)^{1/5} N^{1/5}$, *the MSE bound is asymptotically minimized and*

$$E[(\hat{\theta} - \theta)^2] \le C_1^{4/5} C_2^{1/5} N^{-4/5}.$$

The theorem indicates that the MSE of $\hat{\theta}$ is of order $C_1 n^{-1} + C_2 m^{-4}$, where from the proof of the theorem in Section 3.3 below we see that C_1 is the variance of $\mathbf{X}$ and C_2 is the difference of the expectations of $\mathbf{X}$ under true state $\rho(t_m)$ and the simulated state $\tilde{\rho}(t_m)$. As the Monte Carlo quantum simulation procedure performs n repeated simulations of the quantum system with m state approximations for each simulation, if we have the computational capacity of carrying out a total of $N = mn$ state approximations in the Monte Carlo quantum simulation, the theorem provides optimal strategy for the allocation of m and n that minimizes the MSE of $\hat{\theta}$.

3.3. *Proof of Theorem* 3.1. As usual, the MSE analysis involves deriving its variance and bias,

$$E[(\hat{\theta} - \theta)^2] = \mathrm{Var}(\hat{\theta}) + (E\hat{\theta} - \theta)^2. \tag{10}$$

We need to fix some notation to facilitate further analysis. The target θ is defined under the true final state $\rho(t_m)$, while the quantum simulation is under approximate final state $\tilde{\rho}(t_m)$ which is close to $\rho(t_m)$. To make the problem realistic, we impose the following assumption to ensure that observable $\mathbf{X}$ behaves well in states close to the true final state. With the true final state of the form

$$\rho(t_m) = \sum_{k=1}^{K} p_k |\psi_k(t_m)\rangle\langle\psi_k(t_m)|,$$

we assume that for some small $\eta > 0$

$$\max_{1\le k\le K} \sup\{\|\mathbf{X}|\phi\rangle\|, \||\phi\rangle - |\psi_k(t_m)\rangle\| < \eta\} < \infty. \tag{11}$$

The condition is to ensure that observable $\mathbf{X}$ has two finite moments under states in a small neighborhood of the true state $\rho(t_m)$ of the quantum system.

Since a simple conditional argument will reduce the proof from the general ensemble state case to the pure state case, for simplicity, we consider the Monte Carlo study with pure states. The state used in (8) is the pure state $|\psi(t_m)\rangle$ or

$\rho = |\psi(t_m)\rangle\langle\psi(t_m)|$, under which observable $\mathbf{X}$ and its measurement result X are considered. The measurement results $X_1, \ldots, X_n$ are obtained from the quantum simulation under the simulated state $|\tilde{\psi}(t_m)\rangle$ or $\tilde{\rho} = |\tilde{\psi}(t_m)\rangle\langle\tilde{\psi}(t_m)|$. Therefore, to analyze the bias and variance, we need to evaluate the expectations and variances of X_i under $\tilde{\rho}$ but compute the corresponding quantities of X under ρ.

The bias $E\hat{\theta} - \theta = \mathrm{Tr}(\mathbf{X}\tilde{\rho}) - \mathrm{Tr}(\mathbf{X}\rho)$ is due to the differences between $|\tilde{\psi}(t_j)\rangle$ obtained in the quantum simulation and the true quantum states $|\psi(t_j)\rangle$. We will prove in Proposition 3.1 below

$$\big\||\tilde{\psi}(t_m)\rangle - |\psi(t_m)\rangle\big\| \le C\delta^2. \tag{12}$$

Thus, we derive the bias

$$\begin{aligned} |E\hat{\theta} - \theta| &= |\mathrm{Tr}(\mathbf{X}\tilde{\rho}) - \mathrm{Tr}(\mathbf{X}\rho)| \\ &= \big|\langle\tilde{\psi}(t_m)|\mathbf{X}|\tilde{\psi}(t_m)\rangle - \langle\psi(t_m)|\mathbf{X}|\psi(t_m)\rangle\big| \\ &\le \big|\langle\tilde{\psi}(t_m) - \psi(t_m)|\mathbf{X}|\tilde{\psi}(t_m)\rangle\big| + \big|\langle\tilde{\psi}(t_m)|\mathbf{X}|\tilde{\psi}(t_m) - \psi(t_m)\rangle\big| \\ &\le \big\||\tilde{\psi}(t_m) - \psi(t_m)\rangle\big\|\big(\|\mathbf{X}|\tilde{\psi}(t_m)\rangle\| + \|\mathbf{X}|\psi(t_m)\rangle\|\big) \\ &\le C\delta^2, \end{aligned} \tag{13}$$

where the last inequality is due to (12) and condition (11). The variance of $\hat{\theta}$ is easy to obtain

$$\mathrm{Var}(\theta) = \frac{1}{n}\mathrm{Var}(X_1) = \frac{1}{n}\{\mathrm{Tr}(\mathbf{X}^2\tilde{\rho}) - [\mathrm{Tr}(\mathbf{X}\tilde{\rho})]^2\}. \tag{14}$$

As we have shown above, the $\mathrm{Tr}(\mathbf{X}\tilde{\rho})$ approach to $\theta = \mathrm{Tr}(\mathbf{X}\rho)$ as $m \to \infty$ or, equivalently, $\delta \to 0$. As for $\mathrm{Tr}(\mathbf{X}^2\tilde{\rho})$,

$$|\mathrm{Tr}(\mathbf{X}^2\tilde{\rho})| = |\langle\tilde{\psi}(t_m)|\mathbf{X}^2|\tilde{\psi}(t_m)\rangle| = \|\mathbf{X}|\tilde{\psi}(t_m)\rangle\|^2,$$

whose finiteness is a consequence of (12) and condition (11). Collecting together (10), (13) and (14), we conclude

$$E[(\hat{\theta} - \theta)^2] \le \frac{C_1}{n} + C_2\delta^4 \sim \frac{C_1}{n} + \frac{C_2T^4}{m^4},$$

which is asymptotically minimized when $n \sim m^4 \sim N^{4/5}$. To complete the proof of Theorem 3.1, we show (12) in the rest of the section.

The quantum simulation uses $|\tilde{\psi}(t_j)\rangle$ to approximate the true quantum states $|\psi(t_j)\rangle$ and thus results in approximation errors. We define the following quantity to measure the approximation errors. Suppose U_1 and U_2 are two unitary transformations, the operator norm of the difference between U_1 and U_2,

$$\Gamma(U_1, U_2) = \max_{\|\phi\|=1} \big\|(U_1 - U_2)|\phi\rangle\big\|,$$

is used to measure the closeness of U_1 and U_2.

In the quantum simulation scheme, we approximate $e^{-iHj\delta}$ by U_δ^j defined in (6). Naturally we use $\Gamma(U_\delta^j, e^{-iHj\delta})$ to gauge the approximation errors in the quantum simulation. Below we derive the order in terms of δ for approximation errors $U_\delta^j - e^{-iHj\delta}$ in the quantum simulation.

PROPOSITION 3.1. *The following inequality holds uniformly for* $j = 1, \ldots, m$:

$$\Gamma(U_\delta^j, e^{-iHj\delta}) \le CL\delta^2.$$

PROOF. First we prove the inequality for $j = 1$. For the case of $L = 2$, $H = H_1 + H_2$. Expanding exponential functions of H_i and using simple algebraic manipulation, we have

$$\begin{aligned}
e^{-iH_1\delta/2} &= I - \frac{i}{2}H_1\delta - \frac{1}{8}H_1^2\delta^2 + O(\delta^3),\\
e^{-iH_2\delta} &= I - iH_2\delta - \frac{1}{2}H_2^2\delta^2 + O(\delta^3),\\
e^{-i(H_1+H_2)\delta} &= I - i(H_1+H_2)\delta - \frac{1}{2}(H_1+H_2)^2\delta^2 + O(\delta^3)\\
&= I - i(H_1+H_2)\delta - \frac{1}{2}\delta^2(H_1H_2 + H_2H_1 + H_1^2 + H_2^2) + O(\delta^3)\\
&= \left(I - \frac{i}{2}H_1\delta - \frac{1}{8}H_1^2\delta^2\right)\left(I - iH_2\delta - \frac{1}{2}H_2^2\delta^2\right)\\
&\quad \times \left(I - \frac{i}{2}H_1\delta - \frac{1}{8}H_1^2\delta^2\right) + O(\delta^3)\\
&= e^{-iH_1\delta/2}e^{-iH_2\delta}e^{-iH_1\delta/2} + O(\delta^3) = U_\delta + O(\delta^3).
\end{aligned}$$

For general L, let $H_j^* = \sum_{\ell=j}^L H_\ell$. Then $H = H_1^*$ and $H_j^* = H_j + H_{j+1}^*$ for $j = 1, \ldots, L-1$. We repeatedly apply the above result for the case of $L = 2$ to the case of $H_j^* = H_j + H_{j+1}^*$ and obtain

$$\begin{aligned}
e^{-iH\delta} &= e^{-i(H_1+H_2^*)\delta}\\
&= e^{-iH_1\delta/2}e^{-iH_2^*\delta}e^{-iH_1\delta/2} + O(\delta^3)\\
&= e^{-iH_1\delta/2}e^{-i(H_2+H_3^*)\delta}e^{-iH_1\delta/2} + O(\delta^3)\\
&= e^{-iH_1\delta/2}[e^{-iH_2\delta/2}e^{-iH_3^*\delta}e^{-iH_2\delta/2} + O(\delta^3)]e^{-iH_1\delta/2} + O(\delta^3)\\
&= e^{-iH_1\delta/2}e^{-iH_2\delta/2}e^{-iH_3^*\delta}e^{-iH_2\delta/2}e^{-iH_1\delta/2} + O(2\delta^3)\\
&= \cdots = U_\delta + O(L\delta^3),
\end{aligned}$$

which implies the inequality for $j = 1$.

Second we show the inequality for $j = 2$. Let $V_\delta = e^{-iH\delta}$. For any state $|\phi\rangle$,

$$\begin{aligned}\|(U_\delta^2 - V_\delta^2)|\phi\rangle\| &\le \|(U_\delta^2 - U_\delta V_\delta)|\phi\rangle\| + \|(U_\delta V_\delta - V_\delta^2)|\phi\rangle\| \\ &\le \|U_\delta(U_\delta - V_\delta)|\phi\rangle\| + \|(U_\delta - V_\delta)V_\delta|\phi\rangle\| \\ &\le \|(U_\delta - V_\delta)|\phi\rangle\| + \|(U_\delta - V_\delta)|\phi'\rangle\|,\end{aligned}$$

where $|\phi'\rangle = V_\delta|\phi\rangle$. Since V_δ is unitary, $\||\phi'\rangle\| = \||\phi\rangle\|$. On both sides of the above inequality we take the maximum over all ϕ with $\||\phi\rangle\| = 1$ and obtain

$$\begin{aligned}\Gamma(U_\delta^2, V_\delta^2) &= \max_{\||\phi\rangle\|=1} \|(U_\delta^2 - V_\delta^2)|\phi\rangle\| \\ &\le 2\max_{\phi} \|(U_\delta - V_\delta)|\phi\rangle\| \\ &= 2\Gamma(U_\delta, V_\delta) \le CL\delta^3,\end{aligned}$$

where the last inequality is from the proved case of $j = 1$.

The result for general j follows by induction. Since U_δ and V_δ are unitary, we repeatedly apply the same technique for proving the case of $j = 2$ as follows. For $|\phi\rangle$ with $\||\phi\rangle\| = 1$,

$$\begin{aligned}\|(U_\delta^j - V_\delta^j)|\phi\rangle\| &\le \|(U_\delta^j - U_\delta^{j-1}V_\delta)|\phi\rangle\| + \|(U_\delta^{j-1}V_\delta - V_\delta^j)|\phi\rangle\| \\ &\le \|U_\delta^{j-1}(U_\delta - V_\delta)|\phi\rangle\| + \|(U_\delta^{j-1} - V_\delta^{j-1})V_\delta|\phi\rangle\| \\ &\le \|(U_\delta - V_\delta|\phi\rangle\| + \|(U_\delta^{j-1} - V_\delta^{j-1})|\phi'\rangle\|,\end{aligned}$$

where $|\phi'\rangle = V_\delta|\phi\rangle$. Taking the maximum over all $|\phi\rangle$ with $\||\phi\rangle\| = 1$ on both sides of the above inequality, we get

$$\begin{aligned}\Gamma(U_\delta^j, V_\delta^j) &\le \Gamma(U_\delta, V_\delta) + \Gamma(U_\delta^{j-1}, V_\delta^{j-1}) \le \cdots \le j\Gamma(U_\delta, V_\delta) \\ &\le m\Gamma(U_\delta, V_\delta) \le CL\delta^2,\end{aligned}$$

where the last inequality is from $m\delta = T$ and the proved case of $j = 2$. □

4. An example. There are a few interesting and realistic quantum systems such as the quantum Ising model and simple harmonic oscillator for which some analytic solutions are available [Dziarmaga (2005) and Sakurai (1995)]. In this section we illustrate the Monte Carlo quantum simulation method with simple harmonic oscillator.

4.1. *Three-dimensional isotropic harmonic oscillator.* We consider a quantum system of $d/3$ particles with three-dimensional isotropic harmonic oscillator. This is a d-dimensional quantum system. By using the natural scales of length and energy in terms of particle mass, angular frequency and Planck's constant, we have the following simple expression for the Hamiltonian of the system:

$$H = (\boldsymbol{\Xi}^2 - \boldsymbol{\Delta})/2,$$

where harmonic operator Δ and isotropic multiplication operator $\boldsymbol{\Xi}^2$ are defined as follows:

$$\boldsymbol{\Delta} = \sum_{j=1}^{d} \nabla_j^2, \qquad \boldsymbol{\Xi}^2 = \sum_{j=1}^{d} \boldsymbol{\xi}_j^2, \qquad \nabla_j = \frac{\partial}{\partial x_j},$$

$$[\boldsymbol{\xi}_j f](\mathbf{x}) = x_j f(\mathbf{x}), \qquad \mathbf{x} = (x_1, \ldots, x_d)^\dagger \in \mathbb{R}^d,\ f \in L(\mathbb{R}^d),$$

and for $\ell = 1, \ldots, d/3$, $(x_{3\ell-2}, x_{3\ell-1}, x_{3\ell})$ specify the position coordinates of the ℓth particle in $\mathbb{R}^3$. Hamiltonian H can be written as a sum of d local Hamiltonians $H_j = (\boldsymbol{\xi}_j^2 - \nabla_j^2)/2$. H_j are one-dimensional harmonic oscillators and have expression $H_j = A^+A^- + 1/2$, where A^+ and A^- are creation and annihilation operators given below,

$$A^{\pm} = (\boldsymbol{\xi}_j \mp \nabla_j)/\sqrt{2}, \qquad [A^-, A^+] = A^-A^+ - A^+A^- = I.$$

As shown in Dziarmaga (2005), the Hamiltonian of the quantum Ising model can also be expressed by similar product of creation and annihilation operators.

Operator A^+A^- has eigenvalues k for $k = 0, 1, \ldots$, with eigenfunctions defined by normalized Hermite polynomials,

$$h_k(x) = \frac{(-1)^k}{\sqrt{2^k k! \sqrt{\pi}}} e^{x^2/2} \frac{d^k}{dx^k}(e^{-x^2}). \tag{15}$$

In fact, it can be directly verified that $[x^2 h_k(x) - h_k''(x)]/2 = (k + 1/2)h_k(x)$ and, thus, $h_k(x)$ are eigenfunctions of H_j corresponding to eigenvalues $k + 1/2$. As Hamiltonian H is a sum of d one-dimensional harmonic oscillators, eigenfunctions of Hamiltonian H are given by

$$h_{\vec{k}}(\mathbf{x}) = \prod_{j=1}^{d} h_{k_j}(x_j), \qquad \vec{k} = (k_1, \ldots, k_d)^\dagger, k_j = 0, 1, \ldots,$$

with corresponding eigenvalues $\sum_{j=1}^{d} k_j + d/2$.

4.2. *Quantum simulation*. To make the quantum simulation manageable computationally, we consider the simulation of the following six-dimensional quantum system described by 12 qubits. It requires a Hilbert space of dimension $2^{12} = 4096$ to accommodate the quantum system. We use the first four eigenfunctions of a one-dimensional harmonic oscillator to form two qubit states in each dimension. With the six sets of the four eigenfunctions, we obtain 4096 eigenfunctions of product form and generate a Hilbert space of dimension 4096 to accommodate the 12 qubit quantum system. To define and code the 12 qubits through the eigenfunctions, let $\mathbf{z} = (z_1, \ldots, z_{12})^\dagger$ with $z_j = 0$ or 1, and $\vec{k} = (k_1, \ldots, k_6)^\dagger = (z_1, \ldots, z_6)^\dagger + 2(z_7, \ldots, z_{12})^\dagger$, where $\dagger$ denotes the transpose of a vector. The

coordinates of $\vec{k}$ take four integer values from 0 to 3. We identify qubit state $|z_1 \cdots z_{12}\rangle$ with eigenfunction $h_{\vec{k}}(\mathbf{x})$. The quantum system is governed by Hamiltonian H and evolves in time interval $[0, 1]$. Let $V_\delta = e^{-iH\delta}$. We illustrate the quantum simulation by approximating V_δ with

$$U_\delta = \prod_{j=1}^{6} [e^{-i\xi_j^2 \ell\delta/4} e^{i\nabla_j^2 \ell\delta/2} e^{-i\xi_j^2 \ell\delta/4}].$$

Assume that the quantum system has an initial state at $t_0 = 0$:

$$|\varphi_0\rangle = \frac{1}{64} \sum_{z_j=0}^{1} |z_1 \cdots z_{12}\rangle = \frac{1}{64} \sum_{k_j=0}^{3} h_{k_1}(x_1) \cdots h_{k_6}(x_6),$$

and final true state $|\varphi_m\rangle$ at $t_m = 1$, where for $j = 1, \ldots, m$,

$$|\varphi_j\rangle = e^{-iHt_j} |\varphi_0\rangle = V_\delta^j |\varphi_0\rangle = \frac{1}{64} \sum_{z_j=0}^{1} e^{-i(z_1+\cdots+z_6+2z_7+\cdots+2z_{12}+3)t_j} |z_1 \cdots z_{12}\rangle$$

$$= \frac{1}{64} \sum_{k_j=0}^{3} e^{-i(k_1+\cdots+k_6+3)t_j} h_{k_1}(x_1) \cdots h_{k_6}(x_6).$$

The approximation states in the quantum simulation are

$$|\tilde{\varphi}_j\rangle = U_\delta^j |\varphi_0\rangle, \qquad j = 1, \ldots, m.$$

Consider a path-dependent observable

$$\mathbf{X} = \frac{1}{20} \sum_{z_j=0}^{1} (z_1 + \cdots + z_6 + 2z_7 + \cdots + 2z_{12}) \mathbf{Q}_{e^{-iHt_{z(b)}}|\mathbf{z}\rangle},$$

where $\mathbf{Q}$ is a projection operator, $\mathbf{z} = (z_1, \ldots, z_{12})^\dagger$, $z(b) = \sum_{j=1}^{12} z_j 2^{j-1}$ corresponds to the number with binary representation $z_1 \cdots z_{12}$, and

$$e^{-iHt_{z(b)}} |\mathbf{z}\rangle = e^{-i(z_1+\cdots+z_6+2z_7+\cdots+2z_{12}+3)t_{z(b)}} |z_1 \cdots z_{12}\rangle$$
$$= e^{-i(k_1+\cdots+k_6+3)t_{z(b)}} h_{k_1}(x_1) \cdots h_{k_6}(x_6).$$

We compute $\mathrm{tr}(\mathbf{X}\rho)$ and $\mathrm{tr}(\mathbf{X}^2\rho)$ as follows:

$$\mathbf{X}|\varphi_m\rangle = \frac{1}{20} \sum_{z_j=0}^{1} (z_1 + \cdots + z_6 + 2z_7 + \cdots + 2z_{12})$$
$$\times e^{-i(z_1+\cdots+z_6+2z_7+\cdots+2z_{12}+3)} |z_1 \cdots z_{12}\rangle$$
$$= \frac{1}{20} \sum_{k_j=0}^{3} (k_1 + \cdots + k_6 + 3) e^{-i(k_1+\cdots+k_6+3)} h_{k_1}(x_1) \cdots h_{k_6}(x_6),$$

$$\theta = \operatorname{tr}(\mathbf{X}\rho) = \langle\varphi_m|\mathbf{X}|\varphi_m\rangle = \frac{1}{20\times 2^{12}}\sum_{k_j=0}^{3}(k_1+\cdots+k_6+3) = 0.6,$$

$$\operatorname{tr}(\mathbf{X}^2\rho) = \langle\varphi_m|\mathbf{X}^2|\varphi_m\rangle = \frac{1}{20^2\times 2^{12}}\sum_{k_j=0}^{3}(k_1+\cdots+k_6+3)^2 = 0.37875,$$

$$\operatorname{Var}(\hat{\theta}) = \frac{1}{n}[\operatorname{tr}(\mathbf{X}^2\rho) - \theta^2] = \frac{0.01875}{n}.$$

Hence, we obtain the following expression for the MSE of $\hat{\theta}$:

$$MSE = \frac{0.01875}{n} + (\langle\tilde{\varphi}_m|\mathbf{X}|\tilde{\varphi}_m\rangle - 0.6)^2.$$

We need to numerically compute $\langle\tilde{\varphi}_m|\mathbf{X}|\tilde{\varphi}_m\rangle$ for the MSE evaluation. As H_ℓ and H_j are commutable, $e^{-iHj\delta} = e^{-iH_1 j\delta}\cdots e^{-iH_6 j,\delta}$, and

$$e^{-iHj\delta}h_{k_1}(x_1)\cdots h_{k_6}(x_6) = \prod_{\ell=1}^{6} e^{-iH_\ell j\delta}h_{k_\ell}(x_\ell).$$

The numerical method in Zalka (1998) can be used to evaluate $e^{-iH_\ell j\delta}h_{k_\ell}(x_\ell)$ by repeatedly applying

$$U_\delta h_{k_1}(x_1)\cdots h_{k_6}(x_6) = \prod_{\ell=1}^{6}[e^{-i\xi_\ell^2\delta/4}e^{i\nabla_\ell^2\delta/2}e^{-i\xi_\ell^2\delta/4}h_{k_\ell}(x_\ell)].$$

We approximate $(\langle\tilde{\varphi}_m|\mathbf{X}|\tilde{\varphi}_m\rangle - 0.6)^2$ for $N = 5000$ and δ ranging from 0 to 0.01 and then evaluate MSE. The resulting MSE as a function of δ decreases for δ from 0 to 0.0035 and then starts to increase. Its unique minimum is achieved at $\delta = 0.0035$, which corresponds to $m = 277$ and $n = 18$. Thus, with total 5000 times of state approximations allowed in the Monte Carlo quantum simulation for estimating θ, the Monte Carlo strategy to minimize the MSE of $\hat{\theta}$ is to take $\delta = 0.0035$ in the quantum simulation scheme and repeatedly simulate the quantum system 18 times.

Acknowledgments. The author thanks editor Samuel Kou, the Associate Editor and an anonymous referee for helpful comments and suggestions.

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