Variational quantum simulation of general processes

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Hybrid variational quantum algorithms have been proposed for simulating many-body quantum systems with shallow quantum circuits, and are therefore relevant to Noisy Intermediate Scale Quantum devices. These algorithms are often discussed as a means to solve static energy spectra and simulate the dynamics of real and imaginary time evolutions. Here we consider broader uses of the variational method to simulate general processes. We first show a variational algorithm for simulating the generalised time evolution with a non-hermitian Hamiltonian. Then we consider matrix multiplication, a vital component of diverse applications in many fields including machine learning and optimisation. We first convert matrix multiplication into a matrix evolution problem and show how it can be simulated with the algorithm for generalised time evolution. Meanwhile, when considering matrices that are products of small matrices, we propose an alternative variational algorithm that can realise matrix multiplication with a simpler circuit. Finally, we focus on open quantum systems and apply the developed methods to the variational simulation of stochastic master equations. We numerically test our theory with a single qubit system suffering dephasing noise.

I. INTRODUCTION

Variational algorithms have been invented as a powerful classical tool for efficiently simulating a wide range of many-body quantum systems [1–5]. It has been recently generalised to variational quantum simulation with trial states efficiently prepared by quantum hardware and information extracted from a coherent measurement of the state [6–25]. Different from the conventional quantum simulation algorithms with a universal quantum computer [26–28] that generally requires the coherent control of millions of qubits [29, 30], the trial state in variational quantum algorithms can be prepared with shallow quantum circuits [6, 11, 31–34], which can be robust to a certain amount of device noise and is compatible with near-term Noisy Intermediate Scale Quantum (NISQ) hardware [35]. Variational quantum algorithms can be utilised for efficiently finding energy spectra [7–12, 19, 21–25] and simulating real time Schrödinger evolution of many-body systems [13]. Although quantum circuits are unitary operations, variational algorithm is not limited to energy minimisation and unitary processes and it can be used to simulate dissipative imaginary time evolution that cannot be mapped to unitary gates [20].

In this work, we theoretically study variational quantum simulation and show that it is not limited to these problems. First, we propose a variational quantum algorithm for simulating the generalised time evolution defined by

$$\frac{d}{dt}\left|v(t)\right\rangle = \left|dv(t)\right\rangle, \tag{1}$$

where $|v(t)\rangle$ is the state vector of the target system and $|dv(t)\rangle$ is a sum of states acted upon by arbitrary sparse operators, as we specify following Eq. (17). For example, the real and imaginary time evolution corresponds to the case with $|dv(t)\rangle = -iH|v(t)\rangle$ and $|dv(t)\rangle = (-H - \langle v(t)|H|v(t)\rangle)|v(t)\rangle$, respectively [13, 20]. Therefore, the generalised simulation algorithm can be regarded as a unified framework for simulating general time evolutions. This framework also incorporates non-hermitian quantum mechanics [36–38] that describes nonequilibrium processes [39], parity-time symmetry Hamiltonians [40–42], open quantum systems [43], etc. As we will discuss shortly, the generalised time evolution is also useful for realising general matrix multiplications.

Matrix manipulation is important in many fields including machine learning and optimisation [44, 45]. Various algorithms have been developed for realising matrix manipulation with universal quantum computers [46–50]. In this work, we introduce variational quantum algorithms for simulating matrix multiplications. Consider matrix multiplications that apply a sparse matrix $\mathcal{M}$ to a vector $|v_0\rangle$ as

$$|v\rangle = \mathcal{M}|v_0\rangle, \tag{2}$$

where M is a general non-hermitian matrix that has decomposition $M = \sum_i \lambda_i \sigma_i$ in the Pauli basis and the vector $|v_0\rangle$ is proportional to a quantum state, $|v_0\rangle = \alpha|\psi_0\rangle$. By setting $G = (\mathcal{M} - I)/T$, we can define an evolution of $|v(t)\rangle$ via

$$\frac{\partial}{\partial t}|v(t)\rangle = G|v_0\rangle, \tag{3}$$

with $|v(T)\rangle = \mathcal{M}|v_0\rangle$. As a special case of the generalised time evolution, such a process can be simulated with variational quantum algorithms.

Alternatively, we can also realise matrix multiplication only with variational real and imaginary time evolution by assuming an efficient singular decomposition of $\mathcal{M} = UDV$, with unitary matrices U and V and diagonal matrix D. We can either directly multiply U and V

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if they are simple to realise or simulate it via variational real time evolution [13] if they can be efficiently represented by $e^{-iH^{U(V)}T}$ with sparse Hamiltonian $H^{U(V)}$ and time T. The diagonal matrix D can be realised with variational imaginary time evolution given $D = e^{-H^D T}$ with Hamiltonian H^D [20]. All these assumptions can be naturally fulfilled when $\mathcal{M}$ is a product of matrices that only involves a constant number of qubits. Although this corresponds to the classically tractable case, the state may not be efficiently represented classically and the overall multiplication can be still hard.

Finally, we combine the variational algorithms for simulating the generalised time evolution and matrix multiplication to simulating the evolution of open quantum systems [51–53]. Described by the stochastic master equation (SME), the evolution of the quantum system can be regarded as an average of wave functions that undergo a continuous measurement induced from the environment [53, 54]. The evolution of each wave function is composed of two processes that can be both simulated with variational algorithms: It either continuously evolves under the generalised time evolution with the system Hamiltonian and the damping effect due to continuous measurement; Or the state discontinuously jumps according to the measurement results. The continuous process can be described by Eq. (1) and the jump process is a matrix multiplication process given in Eq. (2). Simulating the evolution of general open quantum systems is of great importance for simulating quantum systems that inevitably interacts with the environment. Existing quantum algorithms [55–60] for simulating open quantum systems generally require deep quantum circuits. As our algorithm is compatible with shallow circuits, it can be realised with NISQ hardware.

This paper is organised as follows. In Sec. II, we review the quantum variational real and imaginary simulation algorithms. In Sec. III, we show our variational algorithm for simulating the generalised time evolution. In Sec. IV, we present two methods to simulate matrix multiplication. In Sec. V, we focus on variational simulation of SME of open quantum systems.

II. VARIATIONAL QUANTUM SIMULATION OF REAL AND IMAGINARY TIME EVOLUTION

We first review the variational quantum algorithms for simulating real and imaginary time evolution introduced in Ref. [13] and [20], respectively. We refer the reader to Ref. [61] for a comprehensive derivation of quantum variational algorithms from various variational principles — the Dirac and Frenkel variational principle, the McLachlan's variational principle, and the time-dependent variational principle. The real time evolution is described by the Schrödinger equation,

$$\frac{d\left|\psi(t)\right\rangle}{dt} = -iH\left|\psi(t)\right\rangle, \tag{4}$$

with hermitian Hamiltonian H. Instead of directly simulating the real time dynamics with the Hamiltonian simulation algorithms [62–66], the variational method assumes that the quantum state $|\psi(t)\rangle$ is prepared by a parametrised quantum circuit, $|\varphi(\vec{\theta}(t))\rangle = R_N(\theta_N)\dots R_k(\theta_k)\dots R_1(\theta_1)\left|\bar{0}\right\rangle$ with each gate $R_k(\theta_k)$ controlled by the real parameter θ_k and the reference state $|\bar{0}\rangle$. Here, we denote $\vec{\theta} = (\theta_1, \theta_2, \dots, \theta_N)$. According to McLachlan's variational principle [67], the real time dynamics of $|\psi(t)\rangle$ can be mapped to the evolution of the parameters $\vec{\theta}(t)$ by minimising the distance between the ideal evolution and the evolution induced of the parametrised trial state,

$$\delta\|(\partial/\partial t + iH)\left|\varphi(\vec{\theta}(t))\right\rangle\| = 0, \tag{5}$$

where $\|\left|\varphi\right\rangle\| = \langle\varphi|\varphi\rangle$ is the norm of $|\varphi\rangle$. The solution is

$$\sum_j M_{k,j}\dot{\theta}_j = V_k, \tag{6}$$

with coefficients

$$\begin{aligned} M_{k,j} &= \frac{\partial\left\langle\varphi(\vec{\theta}(t))\right|}{\partial\theta_k}\frac{\partial\left|\varphi(\vec{\theta}(t))\right\rangle}{\partial\theta_j} + h.c., \\ V_k &= -i\left\langle\varphi(\vec{\theta}(t))\right| H\frac{\partial\left|\varphi(\vec{\theta}(t))\right\rangle}{\partial\theta_k} + h.c. \end{aligned} \tag{7}$$

For imaginary time evolution, the normalised Wick-rotated Shrödinger equation is obtained by replacing $t = i\tau$ in Eq. (4),

$$\frac{d\left|\psi(\tau)\right\rangle}{d\tau} = -(H - \langle H\rangle)\left|\psi(\tau)\right\rangle. \tag{8}$$

Applying a similar procedure for real time evolution, the imaginary time evolution is mapped to the evolution of the parameters via McLachlan's principle,

$$\delta\|(\partial/\partial\tau + H - \langle H\rangle)\left|\varphi(\vec{\theta}(t))\right\rangle\| = 0. \tag{9}$$

The evolution of the parameters is

$$\sum_j M_{k,j}\dot{\theta}_j = C_k, \tag{10}$$

with M given in Eq. (7) and C defined by

$$C_k = -\Re\left(\left\langle\varphi(\vec{\theta}(t))\right| H\frac{\partial\left|\varphi(\vec{\theta}(t))\right\rangle}{\partial\theta_k}\right). \tag{11}$$

The M, V, and C terms can be efficiently measured with quantum circuits. Considering gate based circuits, the derivative of the each parameterised gate can be expressed as

$$\frac{\partial R_k}{\partial\theta_k} = \sum_i g_{k,i}R_k\sigma_{k,i}, \tag{12}$$

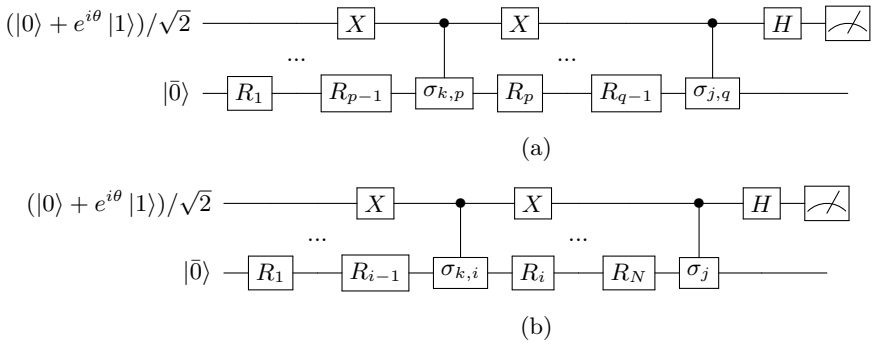

FIG. 1. Quantum circuits that evaluate (a) $\Re(e^{i\theta}\langle\bar{0}|R_{k,p}^\dagger R_{j,q}|\bar{0}\rangle)$ and (b) $\Re(e^{i\theta}\langle\bar{0}|R_{k,i}^\dagger\sigma_j R|\bar{0}\rangle)$.

where $\sigma_{k,i}$ are unitary operators and $g_{k,i}$ are complex coefficients. The derivative of the trial state can be written as

$$\frac{\partial|\varphi(\vec{\theta}(t))\rangle}{\partial\theta_k} = \sum_i g_{k,i}R_{k,i}|\bar{0}\rangle, \tag{13}$$

where

$$R_{k,i} = R_N R_{N-1}\cdots R_{k+1}R_k\sigma_{k,i}\cdots R_2R_1. \tag{14}$$

The $M_{k,j}$ terms can be expressed as

$$M_{k,j} = \sum_{i,j}\Re\left(g_{k,p}^* g_{j,q}\langle\bar{0}|R_{k,p}^\dagger R_{j,q}|\bar{0}\rangle\right). \tag{15}$$

Similarly, considering sparse Hamiltonian with decomposition $H = \sum_j\lambda_j\sigma_j$, $\lambda_j\ \in\mathbb{R}$, we have C_k and V_k as

$$\begin{aligned} V_k &= \sum_{i,j}\Re\left(ig_{k,i}^*\lambda_j\langle\bar{0}|R_{k,i}^\dagger\sigma_j R|\bar{0}\rangle\right), \\ C_k &= -\sum_{i,j}\Re\left(g_{k,i}^*\lambda_j\langle\bar{0}|R_{k,i}^\dagger\sigma_j R|\bar{0}\rangle\right), \end{aligned} \tag{16}$$

All the M, C, and V terms can be written in the form

$$a\Re\left(e^{i\theta}\langle\bar{0}|U|\bar{0}\rangle\right),$$

where $a,\theta\in\mathbb{R}$ depend on the coefficients, and U is a unitary operator of either $R_{k,p}^\dagger R_{j,q}$ or $R_{k,i}^\dagger\sigma_j R$. We can calculate M, C, and V by using the quantum circuit shown in Fig. 1.

III. SIMULATING GENERALISED TIME EVOLUTION

Variational algorithms for real and imaginary time evolutions is to map the original evolution to the evolution of the parameters. It is not hard to see that the variational method is not limited to real or imaginary time evolution. In this section, we extend the idea and propose variational quantum simulation of generalised time evolution,

$$\frac{d}{dt}|v(t)\rangle = |dv(t)\rangle, \tag{17}$$

with $|dv(t)\rangle = \sum_j A_j(t)|v_j'(t)\rangle$. Here, $A_j(t)$ is a time dependent general sparse (non-hermitian) operators $A_j(t) = A_{Rj}(t) + iA_{Ij}(t)$, $|v(t)\rangle$ is the system state, and each of $|v_j'(t)\rangle$ can be either $|v(t)\rangle$ or any known state that can be efficiently prepared with a quantum circuit. The states $|v(t)\rangle$ and $|v_j'(t)\rangle$ can be (un)normalised states $|v(t)\rangle = \alpha(t)|\psi(t)\rangle$, $|v_j'(t)\rangle = \alpha_j'(t)|\psi_j'(t)\rangle$ with normalisation factors $\alpha(t)$ and $\alpha_j'(t)$, and normalised quantum states $|\psi(t)\rangle$ and $|\psi_j'(t)\rangle$, respectively. In practice, we assume that $A(t)_j$ can be decomposed as a linear combination of Pauli operators $A_j(t) = \sum_i\lambda_j^i(t)\sigma_i$ with complex coefficients λ_i and a polynomial (with respect to the system size) number of tensor products of Pauli matrices σ_i.

Considering parameterised quantum states $|v(\vec{\theta}(t))\rangle = \alpha(\vec{\theta}_0(t))|\varphi(\vec{\theta}_1(t))\rangle$, $|v'(\vec{\theta}'(t))\rangle = \alpha'(\vec{\theta}'_{0j}(t))|\varphi'(\vec{\theta}'_{1j}(t))\rangle$ under the McLachlan's principle, we have

$$\delta\|\left(\partial/\partial t|v(\vec{\theta}(t))\rangle - A(t)|v'(\vec{\theta}'(t))\rangle\right)\| = 0. \tag{18}$$

The parameters are $\vec{\theta} := (\vec{\theta}_0,\vec{\theta}_1)$, $\vec{\theta}_j' := (\vec{\theta}'_{0j},\vec{\theta}'_{1j})$ and the solution gives

$$\sum_j\tilde{M}_{k,j}\dot{\theta}_j = \tilde{V}_k \tag{19}$$

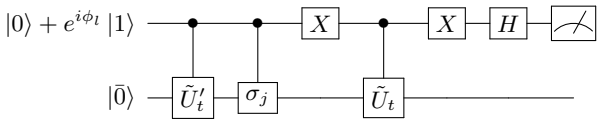

FIG. 2. The quantum circuit for evaluating $\tilde{V}_k$.

with coefficients

$$\begin{aligned}\tilde{M}_{k,j} &= \Re\left(|\alpha(\vec{\theta}_0(t))|^2 \frac{\partial \langle\varphi(\vec{\theta}_1(t))|}{\partial\theta_k}\frac{\partial|\varphi(\vec{\theta}_1(t))\rangle}{\partial\theta_j}\right)\\ &+\Re\left(\frac{\partial\alpha^*(\vec{\theta}_0(t))}{\partial\theta_k}\alpha(\vec{\theta}_0(t))\langle\varphi(\vec{\theta}_1(t))|\frac{\partial|\varphi(\vec{\theta}_1(t))\rangle}{\partial\theta_j}\right)\\ &+\Re\left(\frac{\partial\alpha^*(\vec{\theta}_0(t))}{\partial\theta_j}\alpha(\vec{\theta}_0(t))\langle\varphi(\vec{\theta}_1(t))|\frac{\partial|\varphi(\vec{\theta}_1(t))\rangle}{\partial\theta_k}\right)\\ &+\Re\left(\frac{\partial\alpha(\vec{\theta}_0(t))}{\partial\theta_k}\frac{\partial\alpha^*(\vec{\theta}_0(t))}{\partial\theta_j}\right),\\ \tilde{V}_k &= \Re\left(\frac{\partial\alpha^*(\vec{\theta}_0(t))}{\partial\theta_k}\alpha'(\vec{\theta}'_{0j}(t))\langle\varphi(\vec{\theta}_1(t))|A_j(t)|\varphi'_j(\vec{\theta}'_{1j}(t))\rangle\right).\\ &+\sum_j\Re\left(\alpha^*(\vec{\theta}_0(t))\alpha'(\vec{\theta}'_{0j}(t))\frac{\partial\langle\varphi(\vec{\theta}_1(t))|}{\partial\theta_k}A_j(t)|\varphi'_j(\vec{\theta}'_{1j}(t))\rangle\right).\end{aligned} \tag{20}$$

Each element of the $\tilde{M}$ matrix can be measured with the quantum circuits in Fig. 1. Each term of $\tilde{V}$ can be computed as follows. We denote $\tilde{U}_t$ and $\tilde{U}_t'$ to be the unitary circuit to prepare $|\varphi(\vec{\theta}_1(t))\rangle = \tilde{U}_t|\bar{0}\rangle$ and $|\varphi'_j(\vec{\theta}'_{1j}(t))\rangle = \tilde{U}_t'|\bar{0}\rangle$. Replacing $A_j(t) = \sum_i \lambda_j^i(t)\sigma_i$, the first term of each $\tilde{V}_k$ can be written in a form of $\sum_l a_j\Re\left(e^{i\phi_j}\langle\bar{0}|\tilde{U}_t^\dagger\sigma_j\tilde{U}_t'|\bar{0}\rangle\right)$ with $a_j, \phi_j \in \mathbb{R}$ determined by α, α', and λ. Each term in the summation can be evaluated using the quantum circuit shown in Fig. 2. For the second term of $\tilde{V}_k$, we first represent derivative of the state as in Eq. (13) and then we can compute each term with a similar circuit. Note that when $\tilde{U}$ and $\tilde{U}'$ are not the same, the circuit in Fig. 2 generally doubles the circuit in Fig. 1.

When we simulate the simpler time derivative equation under the condition $|v'(t)\rangle = |v(t)\rangle$,

$$\frac{d}{dt}|v(t)\rangle = A(t)|v(t)\rangle, \tag{21}$$

the term $\tilde{V}_k$ can be obtained by using the same quantum circuit as Fig. 1. We can further consider the normalised evolution described by

$$\frac{d}{dt}|\psi(t)\rangle = (A - \langle A_R\rangle)|\psi(t)\rangle. \tag{22}$$

By applying McLachlan's principle, we get the same evolution Eq. (19) and Eq. (20) with $\alpha(\vec{\theta}_0(t)) = 1$.

Specially, when there is only one term in Eq. (17) with $|v(t)\rangle = |v'(t)\rangle$, it reduces to the real and imaginary time evolution cases with $A = -iH$ and $A = -(H - \langle v(t)|H|v(t)\rangle)$, respectively.

IV. VARIATIONAL MATRIX MULTIPLICATION

Now, we consider matrix multiplication that multiply a sparse square matrix $\mathcal{M}$ to a vector $|v_0\rangle$ as $|v\rangle = \mathcal{M}|v_0\rangle$. Because $\mathcal{M}$ may not be a unitary, we associate a normalisation factor α to quantum states $|\psi\rangle$ to represent the vector $|v\rangle = \alpha|\psi\rangle$. In this section, we present two variational algorithms to realise matrix multiplication.

A. Matrix evolution

The first method is based on the algorithm for simulating generalised time evolution. The idea is to convert matrix multiplication into an genearlised evolution process such that the initial vector $|v_0\rangle$ is evolved to $|v\rangle = \mathcal{M}|v_0\rangle$. The most straightforward evolution path is a linear extrapolation between $|v_0\rangle$ and $|v\rangle$ via

$$|v(t)\rangle = E(t)|v_0\rangle, \tag{23}$$

with

$$E(t) = t/T\cdot\mathcal{M} + \big(1 - t/T\big)I, \tag{24}$$

and $|v(0)\rangle = |v_0\rangle$ and $|v(T)\rangle = |v\rangle$. Different evolution paths can be also considered. For example, in the conventional Hamiltonian simulation scenario, we have $M = e^{-iHT}$ and it corresponds to an exponential extrapolation. We leave the discussion of different choices of the evolution to future works. Given the linear extrapolation between $|v_0\rangle$ and $|v\rangle$, the time derivative equation of $|v(t)\rangle$ is

$$\frac{\partial}{\partial t}|v(t)\rangle = G|v(0)\rangle, \tag{25}$$

with $G = \big(\mathcal{M} - I\big)/T$. This corresponds to setting $A(t) = G$ and $|v'(t)\rangle = |v(0)\rangle$ in the generalised time evolution in Eq. (17). Therefore we can directly apply the variational algorithm proposed in the last section to realise $\mathcal{M}|v(0)\rangle$.

Here, we also consider the case where we are only interested in the normalised final state $|\psi(t)\rangle = \mathcal{M}|v_0\rangle/\sqrt{\|\mathcal{M}|v_0\rangle\|}$. By extrapolating from $|v_0\rangle/\sqrt{\||v_0\rangle\|}$ to $|\psi(t)\rangle$, we can similarly have an evolution of the state $|\psi(t)\rangle$ as

$$|\psi(t)\rangle = E'(t)|\psi_0\rangle, \tag{26}$$

with

$$E'(t) = N(t)\left(\frac{t}{T}\mathcal{M} + (1 - \frac{t}{T})I\right), \tag{27}$$

and a normalisation factor

$$N(t) = \frac{1}{\sqrt{\left\| \left(\frac{t}{T}\mathcal{M} + (1-\frac{t}{T})I \right) |\psi_0\rangle \right\|}}. \quad (28)$$

The normalisation factor $N(t)$ can be measured from the expectation values of $\mathcal{M}^\dagger + \mathcal{M}$ and $\mathcal{M}^\dagger\mathcal{M}$ for $|\psi_0\rangle$. Given the definition of the state $|\psi(t)\rangle$ at time t, the corresponding derivative equation is

$$\frac{d}{dt}|\psi(t)\rangle = \frac{\dot{N}(t)}{N(t)}|\psi(t)\rangle + N(t)G|\psi(0)\rangle. \quad (29)$$

Such an equation is also described by the generalised time evolution equation with $|v(t)\rangle = |\psi(t)\rangle$, $A_1(t) = \frac{\dot{N}(t)}{N(t)}I$, $A_2(t) = N(t)G$, $|v_1'(t)\rangle = |\psi(t)\rangle$ and $|v_2'(t)\rangle = |\psi(0)\rangle$.

B. Singular value decomposition method

Here, we also introduce a second method for realising matrix multiplication with only real and imaginary time evolution. Assumes an efficient singular value decomposition of $\mathcal{M}$ as

$$\mathcal{M} = UDV, \quad (30)$$

with unitary matrices U and V and diagonal matrix D with non-negative entries. Suppose the unitary matrices U and V can be represented by $U = \exp(-iH^U T^U)$ and $V = \exp(-iH^V T^V)$ with time T^U and T^V, respectively, the multiplication of U and V can be realised by evolving the state with Hamiltonian H^U and H^V via variational real time simulation. Given a spectral decomposition of $U = \sum_j e^{i\lambda_j}|\lambda_j\rangle\langle\lambda_j|$ with $\lambda_j \in \mathbb{R}$, we can set $H^U = -\sum_j \lambda_j/T^U |\lambda_j\rangle\langle\lambda_j|$ and similarly for V. To realise the diagonal matrix D, we first define a corresponding Hamiltonian H^D, such that $D \approx \exp(-H^D T^D)$. Suppose $D_k = \sum_j a_j |j\rangle\langle j|$, the Hamiltonian H^D is given by

$$-H^D T = \sum_{a_j \neq 0} \log(a_j)|j\rangle\langle j| + \alpha \sum_{a_j=0} |j\rangle\langle j|, \quad (31)$$

with properly chosen large constant α satisfying $\alpha \gg \log(a_j)$. Therefore, we can define an unnormalised imaginary time evolution

$$\frac{d|v(t)\rangle}{d\tau} = -H^D|v(t)\rangle, \quad (32)$$

so that the initial vector $|v_0\rangle$ is evolved to $D|v_0\rangle$ from $\tau = 0$ to $\tau = T$. Alternatively, we can realised the normalised matrix multiplication $D|v_0\rangle / \|D|v_0\rangle\|$ by considering the normalised imaginary time evolution

$$\frac{d|\psi(t)\rangle}{dt} = -(H^D - \langle H^D(t)\rangle)|\psi(t)\rangle, \quad (33)$$

where $\langle H^D(t)\rangle = \langle\phi(t)| H^D |\phi(t)\rangle$.

Although the second method can realise both unnormalised and normalised matrix multiplication with shorter circuits, it requires the singular value decomposition of $\mathcal{M}$ and expressing the unitary and diagonal matrices with real or imaginary time evolution operators, which is hard for general matrices. However, when considering matrices $\mathcal{M}$ that is a product of matrices that only involve a few qubits, i.e., $\mathcal{M} = \mathcal{M}_1 \otimes \cdots \otimes \mathcal{M}_L$ with $\mathcal{M}_i$ acting on a constant number of qubits, these assumptions can be easily satisfied.

V. VARIATIONAL SIMULATION OF OPEN QUANTUM SYSTEMS

Now, we focus on open quantum systems and apply the variational algorithms to simulate the stochastic mater equation. Note that this approach differs from that in Ref. [61] where we can directly simulate the evolution of the Lindblad master equation however with two copies of the states.

A. Stochastic master equation

Suppose the dynamics of open quantum systems is described by the Lindblad master equation

$$\frac{d}{dt}\rho = -i[H,\rho] + \mathcal{L}\rho. \quad (34)$$

Here, the system Hamiltonian is H and the interaction with the environment $\mathcal{L}\rho$ is described by

$$\mathcal{L}\rho = \sum_k \frac{1}{2}(2L_k\rho L_k^\dagger - L_k^\dagger L_k\rho - \rho L_k^\dagger L_k), \quad (35)$$

with Lindblad operators L_i. Although the Lindblad master equation directly evolves the density matrix, it is equivalent to the stochastic master equation by averaging the trajectory of each pure state evolved under continuous measurements. Because the measurement process is stochastic, the wave function has a stochastic evolution.

Given this Lindblad master equation, the stochastic Schrödinger equation for each single trajectory $|\psi_c(t)\rangle$ is

$$d|\psi_c(t)\rangle = \left(-iH - \frac{1}{2}\sum_{k\geq 1}(L_k^\dagger L_k - \langle L_k^\dagger L_k\rangle)\right)|\psi_c(t)\rangle\, dt + \sum_{k\geq 1}\left(\frac{L_k|\psi_c(t)\rangle}{||L_k|\psi_c(t)\rangle||} - |\psi_c(t)\rangle\right)dN_k, \quad (36)$$

where $d|\psi_c(t)\rangle = |\psi_c(t+dt)\rangle - |\psi_c(t)\rangle$, and dN_k randomly takes either 0 or 1 which satisfies $dN_k dN_{k'} = \delta_{kk'}dN_k$ and $E[dN_k] = \langle\psi_c(t)| L_k^\dagger L_k |\psi_c\rangle\, dt$. With probability $1 - p(t)$ defined below, we have $dN_k = 0$ and the

state evolves under the generalised time evolution with operator

$$A = -iH - \frac{1}{2}\sum_{k\geq 1}(L_k^\dagger L_k - \langle L_k^\dagger L_k\rangle); \tag{37}$$

Here, $-iH$ corresponds to the conventional real time Schrödinger evolution with Hamiltonian H and the rest terms can be understood as a normalised damping process. With probability $p(t)$, we have $dN_k = 1$ and the state discontinuously jumps to $L_k |\psi_c(t)\rangle / \| L_k |\psi_c(t)\rangle \|$, which can be regarded as a measurement with unnormalised Kraus operator L_k. Therefore, the whole process is composed of two parts: the continuous process governed by the first term and the quantum jump process described by the second term. The Lindblad master equation is therefore simulated by averaging different trajectories of $|\psi_c(t)\rangle$ evolving according to the stochastic Schrödinger equation.

We elaborate on more details of the jump process in simulating the stochastic Schrödinger equation. At time t, the jump probability $p(t)$ is given by

$$p(t) = 1 - e^{-\int_0^t \sum_k \langle\psi_c(t')|L_k^\dagger L_k|\psi_c(t')\rangle dt'}, \tag{38}$$

with state $|\psi_c(t')\rangle$ at time t' according to Eq. (36). Then, a random number $q \in [0,1]$ is generated to determine whether jump happens or not. That is, if $q > p(t)$, the state evolves according to the generalised time evolution with operator in Eq. (37). Otherwise, another random number $q' \in [0,1]$ is generated to determine which jump operator to apply. The state is updated to $L_k |\psi_c(t)\rangle / \| L_k |\psi_c(t)\rangle \|$ if $q' \in [\tilde{\gamma}_{k-1}(t), \tilde{\gamma}_k(t)]$, where

$$\tilde{\gamma}_k(t) = \frac{\sum_{l=1}^{k} \langle\psi_c(t)| L_l^\dagger L_l |\psi_c(t)\rangle}{\sum_{l=1}^{N_L} \langle\psi_c(t)| L_l^\dagger L_l |\psi_c(t)\rangle}, \tag{39}$$

and N_L is the number of the Lindblad operators. Considering discretised time with initial state $|\psi_c(0)\rangle$, the stochastic Schrödinger equation from time 0 to T can be simulated as follows.

Algorithm 1 Stochastic Schrödinger equation

1: The jump probability p is initialised to be 0.
2: **for** $n = 1$ to $T/\Delta t$ **do**
3: Generate a random number $q \in [0,1]$, set $t = n\Delta t$.
4: **if** $q > p$ **then**
5: Evolve the state $|\psi_c(t)\rangle$ under A in Eq. (37).
6: Update $p = 1 - e^{-\sum_{j=1}^{n}\sum_k \langle\psi_c(j\Delta t)|L_k^\dagger L_k|\psi_c(j\Delta t)\rangle \Delta t}$.
7: **else**
8: Calculate $\tilde{\gamma}_k(t)$ in Eq. (39)
9: Generate a random number $q' \in [0,1]$.
10: **if** $q' \in [\tilde{\gamma}_{k-1}(t), \tilde{\gamma}_k(t)]$ **then**
11: Update $|\psi_c(t)\rangle$ to $L_k |\psi_c(t)\rangle / \| L_k |\psi_c(t)\rangle \|$.
12: Reset jump probability $p = 0$.

B. Variational quantum algorithms for simulating SML

Now we show how to simulate the Stochastic Schrödinger equation, Algorithm 1, with the variational algorithms developed in this work. Suppose the state $|\psi_c(t)\rangle$ at time t can be represented by the parametrised state $|\phi_c(\vec{\theta}(t))\rangle$ prepared by a quantum computer. We can simulate step 5, i.e., the evolution under operator A Eq. (37), with the algorithm for generalised time evolution. Specifically, we can evolve the parameters according to

$$\sum_j \bar{M}_{k,j}\dot{\theta}_j = \bar{V}_k, \tag{40}$$

with

$$\begin{aligned}\tilde{M}_{k,j} =& \Re\left(\frac{\partial \langle\varphi(\vec{\theta}(t))|}{\partial\theta_k}\frac{\partial |\varphi(\vec{\theta}(t))\rangle}{\partial\theta_j}\right)\\ \tilde{V}_k =& \Re\left(\langle\varphi(\vec{\theta}(t))|(-iH - L)\frac{\partial |\varphi(\vec{\theta}(t))\rangle}{\partial\theta_k}\right),\end{aligned} \tag{41}$$

and $L = \frac{1}{2}\sum_k L_k^\dagger L_k$. The value of $\tilde{\gamma}_k(t)$ at step 8 can be directly calculated from measuring $\langle\psi_c(t)| L_l^\dagger L_l |\psi_c(t)\rangle$. The jump at step 11 can be realised by the variational algorithms for matrix multiplication. Especially, when considering L_k as a product of operators of each qubits, it can be efficiently realised also with the singular value decomposition method. In practice, we consider sparse Hamiltonian and Lindblad operators L, therefore all the measurements can be efficiently evaluated.

C. Example

In this section, we show an example of variational quantum simulation of a single qubit system under dephasing and relaxation process. The stochastic master equation is described by

$$\frac{d}{dt}\rho = -i[\lambda\sigma_x, \rho] + \mathcal{L}_1(\rho) + \mathcal{L}_2(\rho) + \mathcal{L}_3(\rho), \tag{42}$$

with Lindblad terms

$$\begin{aligned}\mathcal{L}_1(\rho) &= D[\sqrt{\gamma_1}|0\rangle\langle 0|](\rho),\\ \mathcal{L}_2(\rho) &= D[\sqrt{\gamma_2}|1\rangle\langle 1|](\rho),\\ \mathcal{L}_3(\rho) &= D[\sqrt{\gamma_3}|0\rangle\langle 1|](\rho),\end{aligned} \tag{43}$$

and

$$D[L](\rho) = \frac{1}{2}(2L\rho L^\dagger - L^\dagger L\rho - \rho L^\dagger L). \tag{44}$$

In our simulation, we set $\lambda = \gamma_1 = \gamma_2 = \gamma_3 = 1$, consider initial state $\rho(0) = |1\rangle\langle 1|$, and simulate the evolution from $t = 0$ to $t = 5$. We parametrised the trial state as

$$|\varphi(\vec{\theta})\rangle = R_x(\theta_1)|0\rangle, \tag{45}$$

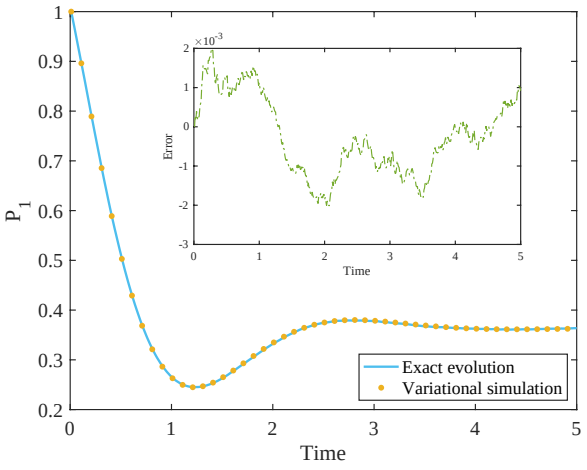

FIG. 3. The comparison between exact evaluation and variational simulation for Eq. (42) from $t = 0$ to $t = 5$. The time step $\delta t = 0.01$. The result of the variational algorithm is averaged over $N_{\text{trial}} = 3.2 \times 10^4$ times. The inset shows the difference of exact evolution and variational simulation.

where $R_x(\theta) = \exp(-i\sigma_x\theta/2)$ is a single qubit rotation operator along the x axis. We can see that set of trial states is only a subspace of the whole Hilbert space of single qubit states.

We simulate the continuous evolution with the variational quantum algorithm for generalised time evolution with $H = \sigma_x$ and $L = |0\rangle\langle 0| + 2|1\rangle\langle 1|$ in Eq. (41). To simulate quantum jumps induced by Lindblad operators, we use the singular value decomposition method. For example, to implement the jump operator $|0\rangle\langle 1|$ corresponding to $\mathcal{L}_3$, we decompose this operator as $|0\rangle\langle 1| = |0\rangle\langle 0| X$. Suppose $|0\rangle\langle 1| = UDV$, we can see that $U = I$, $D = |0\rangle\langle 0|$, $V = X$. To realise the V operator, we set $H_V = X$ and $T_V = \pi/2$ such that $X = \exp(-iH_V T_V)$. Then we evolve the state under Hamiltonian H_V for time T_V with time step $\delta t_V = 0.01$. To realise $D = |0\rangle\langle 0|$, we set $H_D = |1\rangle\langle 1|$ and $T_D = 20$ so that $D \approx \exp(-H_D T_D)$. Then we realise $D|\varphi(\vec{\theta})\rangle$ by using variational imaginary time evolution with total time H_D and time step $\delta t_D = 0.1$. Similarly, for $\mathcal{L}_1$ and $\mathcal{L}_2$, we set $H_D = |1\rangle\langle 1|$ and $|0\rangle\langle 0|$, respectively, and evolve the state under the corresponding Hamiltonian H_D with time $T_D = 20$ and time step $\delta t_D = 0.1$.

In Fig. 3, we show the simulation results that compare between the exact solution of Eq. (42) and the solution obtained from the variational algorithm. We can see that the variational simulation result agrees well with the exact solution.

VI. DISCUSSION

To summarise, we extend the variational quantum simulation method to general processes, including the generalised time evolution, matrix multiplication, and time evolution of open quantum systems. Our algorithm for simulating the generalised time evolution can be applied to simulate non-hermitian quantum mechanics [36–38] including nonequilibrium processes [39] and parity-time symmetry Hamiltonians [40–42]. Especially, it is shown [42] that a quantum state can evolve to the target state faster with non-Hermitian parity-time symmetric Hamiltonians than the case with Hermitian Hamiltonians. Therefore, our variational algorithm for simulating the generalised time evolution may be also useful for designing faster quantum computing algorithms.

Furthermore, the propose algorithms are compatible with NISQ hardware and can be further combined with the recently proposed quantum error mitigation techniques [13, 17, 68–73].

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Appendix A: Derivation of the time derivative equation for parameters for general time derivative equation

Suppose the general time derivative equation to be solved is

$$\frac{d}{dt}\left|v(t)\right\rangle = \sum_j A_j(t)\left|v_j'(t)\right\rangle \tag{A1}$$

By parametrising $|v(t)\rangle$ and $|v_j'(t)\rangle$ as $|v(\vec{\theta}(t))\rangle$ and $|v'(\vec{\theta}_j'(t))\rangle$, with McLachlan's principle, we have

$$\delta\left\|\sum_i \frac{\partial\left|v(\vec{\theta}(t))\right\rangle}{\partial\theta_i}\dot{\theta}_i - \sum_j A_j(t)\left|v'(\vec{\theta}_j'(t))\right\rangle\right\| = 0. \tag{A2}$$

This is equivalent to

$$\begin{aligned}
&\frac{\partial}{\partial\dot{\theta}_k}\left\|\sum_i \frac{\partial\left|v(\vec{\theta}(t))\right\rangle}{\partial\theta_i}\dot{\theta}_i - \sum_j A_j(t)\left|v'(\vec{\theta}_j'(t))\right\rangle\right\| \\
&= \frac{\partial}{\partial\dot{\theta}_k}\left(\sum_i \frac{\partial\left\langle v(\vec{\theta}(t))\right|}{\partial\theta_i}\dot{\theta}_i - \sum_j A_j(t)\left\langle v'(\vec{\theta}_j'(t))\right|\right) \\
&\left(\sum_l \frac{\partial\left|v(\vec{\theta}(t))\right\rangle}{\partial\theta_l}\dot{\theta}_l - \sum_j A_j(t)\left|v'(\vec{\theta}_j'(t))\right\rangle\right) = 0\ \forall k.
\end{aligned} \tag{A3}$$

Hence, we have

$$\begin{aligned}
&\sum_j\left(\frac{\partial\left\langle v(\vec{\theta}(t))\right|}{\partial\theta_k}\frac{\partial\left|v(\vec{\theta}(t))\right\rangle}{\partial\theta_j} + \frac{\partial\left\langle v(\vec{\theta}(t))\right|}{\partial\theta_j}\frac{\partial\left|v(\vec{\theta}(t))\right\rangle}{\partial\theta_k}\right)\dot{\theta}_j \\
&= \sum_j \frac{\partial\left\langle v(\vec{\theta}(t))\right|}{\partial\theta_k}A_j\left|v_j'(\vec{\theta}_j'(t))\right\rangle + h.c
\end{aligned} \tag{A4}$$

By substituting $|v(\vec{\theta}(t))\rangle = \alpha(\vec{\theta_0}(t))\left|\varphi(\vec{\theta}_1(t))\right\rangle$ and $|v'(\vec{\theta}_j'(t))\rangle = \alpha'(\vec{\theta}_{0j}'(t))\left|\varphi(\vec{\theta}_{1j}'(t))\right\rangle$, we have Eq. (19) and Eqs. (20).