Hybrid quantum variational algorithm for simulating open quantum systems with near-term devices

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Abstract

Hybrid quantum-classical (HQC) algorithms make it possible to use near-term quantum devices supported by classical computational resources by useful control schemes. In this paper, we develop an HQC algorithm using an efficient variational optimization approach to simulate open system dynamics under the Noisy-Intermediate Scale Quantum (NISQ) computer. Using the time-dependent variational principle (TDVP) method and extending it to McLachlan TDVP for density matrix which involves minimization of Frobenius norm of the error, we apply the unitary quantum circuit to obtain the time evolution of the open quantum system in the Lindblad formalism. Finally, we illustrate the use of our methods with detailed examples which are in good agreement with analytical calculations.

Keyword: Hybrid quantum-classical algorithm, Time-dependent variational principle, Open quantum system, Near-term devices.

1 Introduction

As we know, real quantum systems are not isolated from their surroundings, but always interact with the environmental degrees of freedom as an open quantum system. These interactions generally lead to dissipation and decoherence, affecting the behavior of the system. Due to the type of interaction and strength of the coupling between the environment and the system, the dynamics of an open quantum system can be divided into two categories; Markovian and non-Markovian. Markovian dynamics (memoryless), which we will review in this paper, can be described by the first-order differential equation when the system interacts weakly with its surroundings and modeled utilizing a dynamical semigroup in Lindblad form. But in non-Markovian dynamics, the memory effects cannot be ignored, and in this case, the information enters the environment and backflow from it. So considering the dynamics of open systems with many degrees of freedom is one of the significant challenges and allows us to a better understanding of the nonequilibrium dynamics of many-body quantum systems. There are well-known numerical and analytical methods for calculating the dynamics of quantum systems, e.g. Time-dependent variational quantum Monte Carlo [G. Carleo and Fabrizio(2012)], Nonequilibrium dynamical mean-field theory [H. Aoki and Werner(2014)], Time-dependent density-matrix renormalization-group [A. J. Daley and Vidal(2004)] , Hierarchy equations of motion (HEOM) [A and J(2005)] and Multi-configuration time-dependent Hartree [H and M(2008)]. However, with the increase in the size of the system, these classical methods are inefficient and take exponential time.

Hybrid variational quantum-classical algorithms are consisting of a relatively low-depth quantum circuit, designed to utilize both quantum and classical resources to solve specific tasks not accessible to traditional classical computers. This method applies to the quantum simulation of many-body systems for a variety of complex problems including, dynamics [Li and Benjamin(2016)], optimization [A. Kandala and Gambetta(2017), A. Peruzzo and O’Brien(2014), E. Farhi and Gutmann(2014), Farhi and Harrow(2016)], quantum chemistry [Alexander J. McCaskey(2019), et. al.(2019)] and so on. The significant benefit of this method is that it gives rise to a setup that can have much
less strict hardware requirements and promising for the near-term application of small quantum computing. The main idea of this method is dividing the problem into two parts that each of performing a single task and can be implemented efficiently on a classical and a quantum computer. Theoretically and experimentally, it has been shown that using near-term quantum devices containing from tens to hundreds of qubits and limited error correction can achieve quantum supremacy. But it is not enough for quantum algorithms to perform more complex calculations in large-scale quantum systems, where HQC algorithms are the best candidate with low sequences of quantum gate operations. Recently, several HQC methods for solving specific optimization tasks have been developed. Two representative variational HQC are the variations quantum eigensolver (VQE) which is a hybrid algorithm to approximate the ground state eigenvalues for chemical systems [A. Kandala and Gambetta(2017), A. Peruzzo and O’Brien(2014)] and the quantum approximate optimization algorithm (QAOA) for finding an approximate solution of an optimization problem [E. Farhi and Gutmann(2014), Farhi and Harrow(2016)].

One of the conventional methods used in most quantum algorithms to simulate the dynamics of quantum systems is commonly referred to as Trotterization, where the Hamiltonian can be decomposed into a sequence of quantum gates and requires many operations to step through the time evolution, e.g., in the single time step, \( O(N) \) gates and \( O(\sqrt{N}) \) depth [Suzuki(1990), Suzuki(1991)]. Another way to calculate system dynamics is based on variational technique, which first assumes the trial state that depends on the controllable parameters, and then we evaluate a state that provides an excellent approximation to the real state by changing the parameters [J. M. Kreula and Jaksch(2016)].

As mentioned, the dynamics of an open system can be described by the master equation, which contains a unitary part under the system’s Hamiltonian and non-unitary components leading to the decoherence and dissipative. In recent years, various efforts have been developed to simulate the evolution of open quantum system developments [Shi-Jie Wei(2016), Zixuan Hu(2020), Nobuyuki Yoshioka(2019)]. Most of these papers require auxiliary qubits for simulation of open systems due to the non-unitary part of dynamics, which is the effect of the system’s interaction with the environment. One of the effective methods to perform time evaluation of many-body systems is the time-dependent variational principle (TDVP), which is obtained from the Dirac-Frenkel variational principle [P.M.A.Dirac(1930), McLachlan(1964), P. W. Langhoff and Karplus(1972)]. This method has many applications in quantum chemistry based on the time-dependent Hartree-Fock theory [Arrighini and Guidotti(1972)] and strongly correlated systems. Recently, Doriol et al. extended the McLachlan TDVP method to the density matrix for open quantum systems based on the Lindblad approach [Joubert-Doriol and Izmaylov1(2015)]. In this paper, we described and analyzed an efficient manner to realize a plan for simulating open system dynamics that were base on the HQC algorithm. This system depends on the TDVP to optimal gradient control iterative that combines the classical and quantum processors. We design a quantum algorithm for the unitary and non-unitary parts of the Markovian dynamics via Liouvillian superoperator by minimization of the Frobenius norm as a cost function up to a small error. We study our method for obtaining the dynamics of open quantum systems in the presence of different quantum noise, which is in good agreement with analytical calculations. The essential constituent of our simulation algorithm is the potentiality to simulate dynamics of open systems on a quantum computer, and it has found critical applications for a great variety of computational tasks, such as nuclear physics, simulating condensed-matter systems, calculating molecular properties, chemical reaction dynamics [Ivan Kassal and Aspuru-Guzik(2011)], and probing quantum effects in biological systems [Neill Lambert(2013)], and probing quantum effects in biological systems [Neill Lambert(2013)].

The paper is organized as follows. In Sec. 2, we briefly introduce the TDVP method for density matrix, and then we propose a hybrid quantum algorithm for simulating the dynamics of an open quantum system. In Sec. 3, presents our numerical results. Finally, Sec. 4 gives the conclusions with further discussion on future works.

## 2 Our Methods

The variational method was first introduced by Dirac [P.M.A.Dirac(1930)] and Frenkel [Frenkel(1934)] in 1930 to approximate the time-dependent Schrödinger equation. In this method, the wavefunction of the system is determined by a set of parameters and the equation of motion of these parameters is obtained using the variational principle. This method has significant applications in hybrid quantum algorithms; e.g., in Ref [Li and Benjamin(2017)], the authors introduced a hy-
brid quantum algorithm for simulating quantum dynamics of closed systems based on variational principle, which can be implemented on NISQ devices. In our approach, we will extend the HQC algorithm to the dynamics of open quantum systems.

2.1 Time-dependent variational methods
The master equation can be described by \( \dot{\rho}(t) = \mathcal{L}(\rho) \), which is a linear and time-local equation for the evaluation of the density matrix in \( d \)-dimensional Hilbert space. \( \mathcal{L} \) is then an linear map usually called Liouvillian superoperator that contains both the unitary and the non-unitary part which results from the interaction between the system and the environment. In this section, we consider evolution of a quantum density matrix \( \rho(t) \) of the form

\[
\rho(t) = \sum_{j=1}^{N} \sum_{k=1}^{N} B_{jk}(t) |\psi_j(t)\rangle \langle \psi_k(t)|
\]

under the Lindbladian operator

\[
\mathcal{L}(\rho) = -i[H, \rho] + \sum_{j=1}^{K} \gamma_j (L_j \rho L_j^\dagger - \frac{1}{2} \{L_j^\dagger L_j, \rho\}).
\]

Here, we maintain the \( N^2 \) coefficients of \( B_{jk} \) in a matrix \( B \) and the pure states \( \{|\psi_k(t)\rangle\}_{k=1}^{N} \) are each prepared with a parametrized quantum circuit. For each \( k \), we have

\[
|\psi_k(t)\rangle = U_k(t) |0\rangle = \prod_{\alpha} U_{k\alpha}(z_{k\alpha}(t)) |0\rangle
\]

where \( z_{k\alpha}(t) \) is the \( \alpha \)-th parameter in the circuit generating \( |\psi_k(t)\rangle \). Note that the states \( \{|\psi_k(t)\rangle\}_{k=1}^{N} \) may not necessarily be orthogonal. The general settings of the HQC algorithm has four stages:

1. Each unitary \( U_{k\alpha} \) in (3) takes the form \( \exp(-iz_{k\alpha} H_{k\alpha}) \) and can be implemented in \( O(1) \) time. Each Hamiltonian term \( H_{k\alpha} \) is a sum of \( O(1) \) terms which are tensor products of Pauli operators.
2. Each parametrized circuit for preparing the states \( \{|\psi_k(t)\rangle\} \) contains at most \( m \) unitary operators \( U_{k\alpha} \).
3. The time dependence of \( z_{k\alpha} \) should be such that \( |\partial z_{k\alpha}/\partial t| \) is bounded by a constant.
4. The Hamiltonian \( H \) in \( \mathcal{L} \) can be rewritten as a linear combination of \( r \) tensor products of Pauli operators. Each Lindblad jump operator \( L_j \) can be expressed as a linear combination of \( s \) tensor products of Pauli operators.

2.1.1 Simulation dynamics via outer-product method
The basic idea of the simulation is that given the state at current time \( t \), determine the state \( t + \Delta t \) according to time-dependent variational principle [McLachlan(1964)], which dictates that the Frobenius norm \( \|\rho - \mathcal{L}(\rho)\| \) must be minimized. This translates to the stationary condition \( \text{Tr}\{\delta \rho (\dot{\rho} - \mathcal{L}(\rho))\} = 0 \), which leads to the Equation of motion for updating the matrix \( B \) and the parameters \( \{z_{k\alpha}\} \) [Joubert-Doriol and Izmaylov(2015)]:

\[
\dot{B} = S^{-1} LS^{-1} - (S^{-1} \tau B + B \tau^\dagger S^{-1})
\]

\[
\dot{z} = C^{-1} \gamma
\]

where \( S \) is the overlap matrix such that \( S_{jk} = \langle \psi_j | \psi_k \rangle \). Here we omit the time dependence of the objects for notational simplicity. The operator \( L \) is such that \( L_{jk} = \langle \psi_j | \mathcal{L}(\rho) | \psi_k \rangle \). \( \tau \) is a matrix with \( \tau_{jk} = \langle \psi_j | \psi_k \rangle \). The second equation in (4) is a linear system for updating the circuit parameters which generate the pure states \( \{|\psi_k\rangle\} \). \( z \) is all \( \{z_{k\alpha}\} \) stored in a vector and the elements
of vector \( \mathcal{Y} \) are also indexed by two indices. Each element of the matrix \( \mathcal{C} \), accordingly, is indexed by four indices. From [Joubert-Doril and Izmaylov(2015)] we have

\[
C_{k\alpha,l\beta} = \left[ \frac{\partial \psi_k}{\partial z_{k\alpha}} \left\{ \frac{\partial \psi_k}{\partial z_{l\beta}} \right\} - \sum_{p,q} [S^{-1}]_{pq} \left\{ \frac{\partial \psi_k}{\partial z_{k\alpha}} \right\} \left\{ \frac{\partial \psi_k}{\partial z_{l\beta}} \right\} \right] \cdot [\mathcal{B}\mathcal{S}\mathcal{B}]_{lk}.
\]

\[
Y_{k\alpha} = \sum_{\ell} \left[ \frac{\partial \psi_k}{\partial z_{k\alpha}} \langle \mathcal{L}(\rho) | \psi_{\ell} \rangle - \sum_{p,q} [S^{-1}]_{pq} \left\{ \frac{\partial \psi_k}{\partial z_{k\alpha}} \right\} \langle \psi_q | \mathcal{L}(\rho) | \psi_{\ell} \rangle \right] \cdot B_{lk}.
\]

To estimate the resource needed for implementing the simulation scheme, we consider both the cost of computing the objects in Equation 4 as well as the cost of solving Equation 4. The latter cost can be estimated as \( O(N^3 m^3) \) since the matrix \( \mathcal{C} \) is \( (Nm) \times (Nm) \) and the cost of inverting \( \mathcal{C} \) dominates over that of the equation of motion for \( \mathcal{B} \). The cubic scaling assumes Gaussian elimination for solving the linear systems. We then proceed by considering the resource needed for computing each of the quantities on the right-hand side of Equation 4.

**Compute \( S^{-1} \).** Each element of \( S \) is an overlap \( \langle \psi_j | \psi_k \rangle = \langle 0 | U_j^\dagger U_k | 0 \rangle \). Since the circuits for preparing each pure state \( | \psi_k(t) \rangle \) is known, one could evaluate the real and imaginary parts of the overlap \( \langle \psi_k(t) | \psi_{\ell}(t) \rangle \) with simple quantum circuits [Buhrman et al.(2001)Buhrman, Cleve, Watrous, and de Wolf, Chamorro-Posada and Garcia-Escartin(2017)]. The cost for evaluating each element of \( S \) up to error \( \epsilon \) is then \( O(m/\epsilon^2) \), leading to a cost for computing the entire \( S \) to be \( O(N^2 m^2/\epsilon^2) \). Inverting \( S \) costs \( O(N^3) \) via Gaussian elimination. Hence the total cost of computing \( S^{-1} \) is \( O(N^3 + N^2 m^2/\epsilon^2) \).

**Compute \( \tau \).** Each element of \( \tau \) is \( \tau_{k\ell} = \langle \psi_k | \dot{\psi}_{\ell} \rangle \). Here \( \dot{\psi}_{\ell} \) is the time derive of the state \( | \psi_{\ell} \rangle \).

More explicitly,

\[
| \dot{\psi}_{\ell} \rangle = \sum_{\alpha} \left[ \prod_{l=1}^{N} \frac{\partial U_{l(\alpha)}(t)}{\partial z_{l\alpha}} \frac{\partial U_{l(\alpha-1)}(t)}{\partial z_{l\alpha}} \cdots \right] | 0 \rangle.
\]

Note that \( \frac{\partial U_{l\alpha}}{\partial z_{l\alpha}} \) is a scalar and \( \frac{\partial U_{l\alpha}}{\partial t} = -iH_{l\alpha}U_{l\alpha} \) from the general setting discussed above. Hence we have

\[
\tau_{k\ell} = \langle \psi_k | \dot{\psi}_{\ell} \rangle = -i \sum_{\alpha} \left[ \prod_{l=1}^{N} \frac{\partial U_{l\alpha}(t)}{\partial t} \right] \langle 0 | U_k^\dagger \left[ \prod_{l=1}^{N} H_{l\alpha}U_{l\alpha} \right] | 0 \rangle.
\]

Here each term in the bracket can be estimated by first decomposing \( H_{\alpha} \) into tensor products of Pauli operators. From the general setting there are at most \( O(1) \) number of those terms. Each of such Pauli terms can be estimated with circuits of the same form as those computing \( S_{j\ell} \), which costs \( O(m/\epsilon^2) \) to estimate up to error \( \epsilon \). Hence each term in the bracket in (7) costs \( O(m/\epsilon^2) \). Since estimating a sum of \( M \) terms with variance \( O(1) \) to error \( \epsilon \) requires \( O(M^2/\epsilon^2) \) state preparation and measurements [McClean et al.(2016)McClean, Romero, Babbush, and Aspuru-Guzik], to compute \( \tau_{k\ell} \) costs in total \( O(m^2/\epsilon^2) \). Computing the entire \( \tau \) therefore costs \( O(N^2 m^2/\epsilon^2) \).

**Compute \( \mathcal{L} \).** Each element of \( \mathcal{L} \) is \( L_{k\ell} = \langle \psi_k | \mathcal{L}(\rho) | \psi_{\ell} \rangle \). Substituting Equations 1 and 2 into the definition of \( L_{k\ell} \), we have

\[
L_{k\ell} = -i \sum_{p,q} B_{pq} \left( \mathcal{S}_{qp} \langle \psi_k | H | \psi_p \rangle - \mathcal{S}_{kp} \langle \psi_q | H | \psi_k \rangle \right) - \sum_j \sum_{p,q} \tau_{j \ell} \sum_{p,q} B_{pq} \left( \langle \psi_k | L_j^\dagger | \psi_p \rangle \langle \psi_q | L_j^\dagger | \psi_k \rangle - \frac{1}{2} \left( \mathcal{S}_{qp} \langle \psi_k | L_j^\dagger \rangle \langle \psi_p | L_j | \psi_k \rangle + \mathcal{S}_{kp} \langle \psi_q | L_j^\dagger \rangle \langle \psi_l | L_j | \psi_k \rangle \right) \right).
\]

Note that \( L_{k\ell} \) is computed from three types of terms: 1) \( \langle \psi_j | H | \psi_k \rangle \), which costs in total \( O(N^2 m^2/\epsilon^2) \) measurements to estimate to error \( \epsilon \); 2) \( \langle \psi_k | L_j | \psi_{\ell} \rangle \), which costs in total \( O(N^2 m^2/\epsilon^2) \) measurements to estimate within error \( \epsilon \); 3) \( \langle \psi_k | L_j^\dagger | \psi_{\ell} \rangle \) terms, which costs in total \( O(N^2 m^4/\epsilon^2) \) to estimate within error \( \epsilon \). Once these three sets of terms are computed, all matrix elements \( L_{k\ell} \) can be computed easily. Since each \( L_{k\ell} \) contains \( O(N^2) \) terms, the cost of computing the three types of terms is \( O(N^6 m^2 (2^2 + s^2)/\epsilon^2) \) to guarantee variance in estimating \( L_{k\ell} \) under \( \epsilon^2 \). Once these three types of terms are computed, putting together the matrix \( \mathcal{L} \) costs \( O(N^4 s) \) time, which is of much lower order. Therefore the cost of computing \( \mathcal{L} \) is \( O(N^6 m^2 (2^2 + s^2)/\epsilon^2) \).

**Computing \( \mathcal{C} \).** From Equation (5) we see that there are two sets of terms that need to be evaluated:
1. Overlap terms of the form \( \langle \frac{\partial \psi}{\partial z_{k\alpha}} | \frac{\partial \psi}{\partial z_{\ell\beta}} \rangle \). Clearly if \( H_{k\alpha} \) and \( H_{\ell\beta} \) can be expanded into \( O(1) \) terms which are tensor products of Pauli operators, the overlap term consists of \( O(1) \) measurable quantities. Each quantity requires \( O(m/\epsilon^2) \) measurements to estimate up to error \( \epsilon \). Then estimating a single overlap costs \( O(m/\epsilon^2) \), leading to the total cost of estimating the overlap terms \( O(N^2 m^2/\epsilon^2) \).

2. Overlap terms of the form \( \langle \frac{\partial \psi}{\partial z_{k\alpha}} | \psi_p \rangle \). The analysis is similar to above, except that now there are only \( O(N^2 m) \) such terms to evaluate, leading to a total cost of \( O(N^2 m^2/\epsilon^2) \).

Because each \( C_{k\alpha,\ell\beta} \) element contains \( O(N^2) \) terms, the total cost of estimating the matrix element to error \( \epsilon \) is \( O(N^6 m^3/\epsilon^2) \). The total cost of computing \( C \) is then \( O(N^8 m^5/\epsilon^2) \).

3 Numerical example

This section of the paper gives illustrative numerical examples of the performance of the HQC algorithm to dynamics of open systems. For simulating of open system dynamics via outer-product method: First, we generate an initial state \( |\psi(z_{k\alpha}(0))\rangle \) with a sequence of gates parameterized by a unitary quantum circuit and contains set of control parameters \( \{z_{k\alpha}(0)\} \) to be optimized on the quantum processor. Then, we solve the differential Eq.(4) numerically via the classical computer, in which the matrices \( C, Y, S, L \) and \( \tau \) in the equation are evaluated using the sequences of unitary quantum operations in quantum computer. Second, by using the solution, we can project parameters forward by a small-time \( \delta t \) and with the iteration the parameters of \( z_{k\alpha}(t) \) are determined iteratively given their initial values. We show in the Fig. 4 a possible implementation of quantum circuit to obtain the dynamics of an open system that includes different layers for measuring different matrices via outer-product method.

![Figure 1: HQC algorithm for solving quantum dynamics via the outer product method. The task of the classical computer is to determine \( z_{k\alpha} \) parameters and quantum computer evaluate quantum state.](image)

To demonstrate our method, we implemented numerical examples for different open systems. Dephasing noise. For the dephasing process (with the rate \( \gamma \)) that destroys the phase coherence of any superposition, we consider simulating the dynamics of the density matrix which is modeled by a Markovian master equation of

\[
\dot{\rho}(t) = -i[H_s, \rho] + \gamma \sigma_z \rho \sigma_z^\dagger - \frac{\gamma}{2} \sigma_z^\dagger \sigma_z \rho - \frac{\gamma}{2} \rho \sigma_z^\dagger \sigma_z,
\]  

(9)
where $\sigma_z$ is Pauli matrix and $H_s$ is Hamiltonian of system. By considering the $H_s = \frac{\omega_0}{2} \sigma_z$ and initial state $\rho_0 = |\psi\rangle\langle\psi|$ with $|\psi\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$, then evaluating the Eq.(9) leads to time evolution of $\rho(t)$. We suppose $|\psi_1\rangle = e^{i\sigma_z z_1} |0\rangle$ and $|\psi_2\rangle = e^{i\sigma_z z_2} |1\rangle$, and by using Eq.(4) and Eq.(5) we can obtain elements of $L_{kl}$, $S$, $C_{k\alpha,l\beta}$ and $Y_{k\alpha}$. We use expectation value of Pauli matrix $\sigma_x$ that defined as $\langle \sigma_x \rangle = \text{Tr}(\rho \sigma_x)$ for calculation the effect of dephasing process on phase coherence system. Output of hybrid quantum-classical algorithm compared it to exact solution $\langle \sigma_x \rangle$ as shown in Fig. [2].

Figure 2: Value $\langle \sigma_x \rangle$ in the two cases exact and hybrid method. Initial parameters are $\gamma = 1.5$, $z_1 = z_2 = 1$ and $B_{11} = B_{22} = 1$, $B_{12} = B_{21} = 1$

**Dissipative noise.** We consider dissipative dynamics of the open quantum system which is described by following master equation

$$\dot{\rho}(t) = -i[H_s, \rho] + \Gamma \sigma^- \rho \sigma^+ - \frac{\Gamma}{2} \sigma^+ \sigma^- \rho - \frac{\Gamma}{2} \rho \sigma^+ \sigma^-,$$

where $\Gamma$ is dissipation rate and $\sigma^-$ and $\sigma^+$ are raising and lowering operators, respectively. Here, we suppose $H_s = \frac{\omega_0}{2} \sigma_z$, $\rho_0 = |0\rangle\langle 0 |$, $|\psi_1\rangle = e^{i\sigma_z z_1} |0\rangle$ and $|\psi_2\rangle = e^{i\sigma_z z_2} |1\rangle$. We investigate the effect of the dissipation process on the energy system with defining $E = \text{Tr}(\rho H)$. The result of the hybrid quantum-classical algorithm compared it to the exact solution $E$ as indicated in Fig. [3].
Two-level system coupled to a photon mode. We consider a simple harmonic oscillator connected to the Two-level system (TLS) as a closed system that coupling to a reservoir [Bhattacharya et al. (2012) Bhattacharya, Stoutimore, Osborn, and Mizel].

A Hamiltonian that represents the TLS–oscillator system is given by

\[ H = \hbar \omega_r a^\dagger a + \frac{\hbar \omega_r}{2} \sigma_z + G (a \sigma^+ + a^\dagger \sigma^-), \quad (11) \]

where \( \hbar \) is Planck’s constant, \( a \) and \( a^\dagger \) are annihilation and creation operators respectively, which together obey the bosonic commutation and \( G \) is coupling strength. Here \( \sigma^- \) and \( \sigma^+ \) are raising and lowering operators, respectively. This is the Jaynes–Cummings Hamiltonian [Jaynes and Cummings (1963)] and for which the eigenenergy and eigenstates can be obtained analytically [Gerry et al. (2005) Gerry, Knight, and Knight].

The master equation describes the TLS–oscillator system interaction with reservoir given with

\[ \dot{\rho}(t) = -i[H, \rho] + \frac{\gamma}{2} (2\rho \sigma^+ \sigma^- - \sigma^+ \rho \sigma^- - \rho \sigma^+ \sigma^-). \quad (12) \]

We can obtain oscillator photon number the excited and ground-state populations of the TLS by numerically solving Eq. (12). In the case of quantum computing, qubits are computational basis, so we first mapped Hamiltonian into qubits. We use the basis of harmonic oscillator eigenstates, as these can be easily mapped to qubits [SOMMA et al. (2003) SOMMA, ORTIZ, KNILL, and GUBERNATIS]. By considering the truncated eigenstates with the lowest \( d \) energies \( |s\rangle \) and employ binary representation we can encode \( |s\rangle \) to qubits [McARDLE et al. (2019) McARDLE, MAYOROV, SHAN, BENJAMIN, and YUAN]. Therefore \( |s\rangle = |b_k\rangle |b_{k-2}\rangle ... |b_0\rangle \) where \( s = b_k 2^{k-1} + b_{k-2} 2^{k-2} + ... b_0 2^0 \). The representation of the creation operator is

\[ a^\dagger = \sum_{s=0}^{d-2} \sqrt{s + 1} |s + 1\rangle \langle s|, \quad (13) \]

and the annihilation operator can be obtained by taking the Hermitian conjugate of \( a^\dagger \). We can map these binary projectors to Pauli operators

\[
\begin{align*}
|0\rangle \langle 0| &= \frac{1}{2} (I + \sigma_z) \\
|1\rangle \langle 1| &= \frac{1}{2} (I - \sigma_z) \\
|0\rangle \langle 1| &= \frac{1}{2} (\sigma_z + i \sigma_y) \\
|1\rangle \langle 0| &= \frac{1}{2} (\sigma_z - i \sigma_y)
\end{align*}
\quad (14)
\]
Now back to the first problem, here we consider.

|ψ₁⟩ = e^{iσ_1 z_1} e^{ia_1 a^\dagger_1} |n⟩_h |0⟩_s,

and

|ψ₂⟩ = e^{iσ_2 z_2} e^{ia_2 a^\dagger_2} |n⟩_h |1⟩_s,

where h and s refer to harmonic oscillator and TLS, respectively. By considering n=2 that is photon number in the oscillator and using Eq.(13) and binary representation |ψ₁⟩ and |ψ₂⟩ can be mapped to qubit form

|ψ₁⟩ = e^{iσ_1 z_1} e^{I_1 ⊗ I_2} e^{iσ_2 ⊗ I_2} |00⟩,

|ψ₂⟩ = e^{iσ_2 z_2} e^{I_1 ⊗ I_2} e^{iσ_2 ⊗ I_2} |01⟩.

Here we obtain oscillator photon number that define \langle N ⟩ = Tr(ρ_N) where \( N = a^\dagger a \). The numerical results shows in the Fig. [4].

Figure 4: Oscillator photon number in two cases exact and hybrid method. Value of initial parameters are \( z_1 = 0, z_2 = 0 \) and \( B_{11} = B_{12} = B_{21} = B_{22} = 1 \) and \( γ = 10, G = 2 \). Here the somewhat deviation is at only two points, and the other points have compatible with the exact calculation and value error is \( (2 ± 2) \times 10^{-2} \). The error of variational data come from the system calculation errors depend on number of repetitions and initial value of parameters.

**Linear vibronic coupling model.** We consider the linear vibronic coupling model of crossing surfaces. The system contains two electronic states donor |D⟩ and acceptor |A⟩, that coupled through two nuclear [Joubert-Doriot and Izmaylov(2015), Domeke et al.(2004)Domeke, Yarkony, et al., Domecke and Yarkony(2012)].

A Hamiltonian that describes this system given by

\[ H = \sum_{i=1}^{2} \frac{\omega_i}{2} (p_i^2 + x_i^2) \langle |D⟩⟨D| + |A⟩⟨A| - dx_1 \langle |D⟩⟨D| - |A⟩⟨A| + cx_2 \langle |D⟩⟨A| + |A⟩⟨D|, \]

where \( \omega_i \) is the frequency of the coordinate \( x_i \), and \( d \) and \( c \) are coupling constants. The dissipative part is described through the bilinear coupling of the system coordinates \( x_i \) with coordinates of harmonic bath oscillators. The master equation that describes the effect of dissipative dynamics given in Lindblad form

\[ \mathcal{L}(\rho) = -i[H, \rho] + h_1 \sum_i^2 (2L_i^\dagger \rho L_i - L_i^\dagger L_i^\dagger \rho - \rho L_i^\dagger L_i) + h_2 \sum_i^2 (2L_i^\dagger \rho L_i - L_i^\dagger L_i^\dagger \rho - \rho L_i^\dagger L_i), \]

where \( h_1 \) and \( h_2 \) are coupling constants, and \( L_i \) are Lindblad operators that defined as

\[ L_1 = (a_1 - \frac{d}{\omega_1 \sqrt{2}}) |D⟩⟨D| + (a_1 + \frac{d}{\omega_1 \sqrt{2}}) |A⟩⟨A|, \quad L_2 = a_2 (|D⟩⟨D| + |A⟩⟨A|, \]

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where \( a_j = (x_i + ip_j)/\sqrt{2} \) are annihilation operators. In the hybrid method, we need to transform Hamiltonian to qubit form. To this end by setting the system contains two electronic states as a two-level system and \( |D\rangle = |0\rangle \) and \( |A\rangle = |1\rangle \) and \( a^\dagger a = p^2 + x^2 \) we obtain

\[
H = \sum_{i=1}^{2} \frac{\omega_i}{2} (a_i^\dagger a_i) - d(a_1^\dagger + a_1)\sigma_z + c(a^\dagger + a)\sigma_x.
\]  
(19)

This Hamiltonian describes the two harmonic oscillators is coupled with a two-level system (TLS) and the dissipative part is introduced coupling of the system with reservoir. The schematic of this system as shown in Fig. [5]. Similar Example 3 we employ binary representation for mapping Hamiltonian to qubit form. Note that, also Lindblad operators mapping to qubit form. So by considering

\[
|\psi_1\rangle = e^{i\sigma_z z_1} e^{i \sum_{j=1}^{2} l_j^1 \otimes l_j^2} e^{i \sum_{j=1}^{2} l_j^1 \otimes \sigma_j^1} e^{i \sum_{j=1}^{2} l_j^1 \otimes \sigma_j^2} |00\rangle|00\rangle|0\rangle,
\]

\[
|\psi_2\rangle = e^{i\sigma_z z_2} e^{i \sum_{j=1}^{2} l_j^1 \otimes l_j^2} e^{i \sum_{j=1}^{2} l_j^1 \otimes \sigma_j^1} e^{i \sum_{j=1}^{2} l_j^1 \otimes \sigma_j^2} |00\rangle|00\rangle|1\rangle.
\]  
(20)

Here we obtain expectation value of Pauli matrix \( \sigma_z \) that given by \( \langle \sigma_z \rangle = Tr(\rho \sigma_z) \) for study losing energy of TLS. The exact and hybrid solution comparing and results show in the Fig. [5].

**Figure 5:** A schematic of the system described in Example 4. The two harmonic oscillators are coupled a TLS with strenght d and c and coupled to reservoir whit strength h

**Figure 6:** Value \( \sigma_z \) in the two cases exact and hybrid method. Initial parameters are \( h_1 = 1, h_2 = 0, \omega_1 = \omega_2 = 0.007,d = 0.05, c = 0.04 \) and \( z_1 = z_2 = 0 \) and \( B_{11} = B_{22} = B_{12} = B_{21} = 1 \)
4 Conclusion

Using a novel quantum gate model, we have developed a HQC algorithm in near-term quantum resources to dynamics of open systems described by a master equation with generator $L$ in Lindblad form. We have used the time-dependent variational principle to density matrix formalism involves minimization of the Frobenius norm of the error. We compare the analytical and numerical results obtained from the exact solution of the master equation with the HQC algorithm given by outer-product methods by several different examples for fermionic and bosonic environments which are in good agreement with each other. In the future, we will extend these results to the non-Markovian dynamics of open systems.

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References

[A and J(2005)] Ishizaki A and Tanimura Y J. Quantum dynamics of system strongly coupled to low-temperature colored noise bath: Reduced hierarchy equations approach. J. Phys. Soc. Japan, 74(3131), 2005.

[A. J. Daley and Vidal(2004)] U. Schollwöck A. J. Daley, C. Kollath and G. Vidal. Time-dependent density-matrix renormalization-group using adaptive effective hilbert spaces,. J. Stat. Mech., (4005), 2004.

[A. Kandala and Gambetta(2017)] K.Temme M. Takita M. Brink J.-M. Chow A. Kandala, A. Mezzacapo and J. M. Gambetta. A variational eigenvalue solver on a photonic quantum processor. Nature, 549:242, 2017.

[A. Peruzzo and O’Brien(2014)] P. Shadbolt M. Yung X. Zhou P. J. Love A. Aspuru-Guzik A. Peruzzo, J. McClean and J. L. O’Brien. A variational eigenvalue solver on a photonic quantum processor. Nat. Commun., 5:4213, 2014.

[Alexander J. McCaskey(2019)] Jacek Jakowski Shirley V. Moore Titus D. Morris Travis S. Humble Raphael C. Pooser Alexander J. McCaskey, Zachary P. Parks. Quantum chemistry as a benchmark for near-term quantum computers. npj Quantum Information., 5(99), 2019.

[Arrighini and Guidotti(1972)] G. Arrighini and C. Guidotti. Excitation energies from time-dependent hartree-fock calculations. Mol. Phys., 24(631), 1972.

[Bhattacharya et al.(2012)] Bhattacharya, Stoutimore, Osborn, and Mizel M Bhattacharya, MJA Stoutimore, KD Osborn, and Ari Mizel. Understanding the damping of a quantum harmonic oscillator coupled to a two-level system using analogies to classical friction. American Journal of Physics, 80(9):810–815, 2012.

[Buhrman et al.(2001)] Buhrman, Cleve, Watrous, and de Wolf Harry Buhrman, Richard Cleve, John Watrous, and Ronald de Wolf. Quantum fingerprinting. Physical Review Letters, 87(16):167902, 2001. ISSN 0031-9007. doi: 10.1103/PhysRevLett.87.167902. URL http://link.aps.org/doi/10.1103/PhysRevLett.87.167902.

[Chamorro-Posada and Garcia-Escartín(2017)] P Chamorro-Posada and J C Garcia-Escartín. The SWITCH test for discriminating quantum evolutions. 2:1–5, 2017. URL https://arxiv.org/pdf/1706.06564.pdf.

[Domcke and Yarkony(2012)] Wolfgang Domcke and David R Yarkony. Role of conical intersections in molecular spectroscopy and photoinduced chemical dynamics. Annual review of physical chemistry, 63:325–352, 2012.

[Domcke et al.(2004)] Domcke, Yarkony, et al.] Wolfgang Domcke, David Yarkony, et al. Conical intersections: electronic structure, dynamics & spectroscopy, volume 15. World Scientific, 2004.

[E. Farhi and Gutmann(2014)] J. Goldstone E. Farhi and S. Gutmann. A quantum approximate optimization algorithm. arXiv:1411.4028., 2014.
[et. al.(2019)] Yudong Cao et. al. Quantum chemistry in the age of quantum computing. *Chem. Rev.*, 19(119), 2019.

[Farhi and Harrow(2016)] E. Farhi and A. W. Harrow. Quantum supremacy through the quantum approximate optimization algorithm. *arXiv:1602.07674*, 2016.

[Frenkel(1934)] Jakov Frenkel. Wave mechanics: Advanced general theory. 1934.

[G. Carleo and Fabrizio(2012)] M. Schiró G. Carleo, F. Becca and M. Fabrizio. Localization and glassy dynamics of many-body quantum systems. *Sci. Rep.*, 2(243), 2012.

[Gerry et al.(2012)Gerry, Knight, and Knight] M. Schiró G. Carleo, F. Becca and M. Fabrizio. Localization and glassy dynamics of many-body quantum systems. *Sci. Rep.*, 2(243), 2012.

[Gerry et al.(2005)Gerry, Knight, and Knight] M. Schiró G. Carleo, F. Becca and M. Fabrizio. Localization and glassy dynamics of many-body quantum systems. *Sci. Rep.*, 2(243), 2012.

[H and M(2008)] Wang H and Thoss M. From coherent motion to localization: dynamics of the spin-boson model at zero temperature. *New J. Phys.*, 10(115005), 2008.

[H. Aoki and Werner(2014)] M. Eckstein M. Kollar T. Oka H. Aoki, N. Tsuji and P. Werner. Nonequilibrium dynamical mean-field theory and its applications. *Rev. Mod. Phys.*, 86(779), 2014.

[Ivan Kassal and Aspuru-Guzik(2011)] Alejandro Perdomo-Ortiz Man-Hong Yung Ivan Kassal, James D. Whitfield and Alán Aspuru-Guzik. Simulating chemistry using quantum computers. *Annu. Rev. Phys. Chem.*, 62:185, 2011.

[J. M. Kreula and Jaksch(2016)] S. R. Clark J. M. Kreula and D. Jaksch. Non-linear quantum-classical scheme to simulate non-equilibrium strongly correlated fermionic many-body dynamics. *Sci. Rep.*, 6(32940), 2016.

[Jaynes and Cummings(1963)] Edwin T Jaynes and Frederick W Cummings. Comparison of quantum and semiclassical radiation theories with application to the beam maser. *Proceedings of the IEEE*, 51(1):89–109, 1963.

[Joubert-Doriol and Izmaylov(2015)] Loïc Joubert-Doriol and Artur F. Izmaylov. Problem-free time-dependent variational principle for open quantum systems. *J. Chem. Phys.*, 142:134107, 2015.

[Joubert-Doriol and Izmaylov(2015)] Loïc Joubert-Doriol and Artur F. Izmaylov. Problem-free time-dependent variational principle for open quantum systems. *Journal of Chemical Physics*, 142(13):1–9, 2015. ISSN 00219606. doi: 10.1063/1.4916384.

[Li and Benjamin(2016)] Ying Li and Simon C. Benjamin. Efficient variational quantum simulator incorporating active error minimisation. pages 1–12, 2016. URL http://arxiv.org/abs/1611.09301.

[Li and Benjamin(2017)] Ying Li and Simon C Benjamin. Efficient variational quantum simulator incorporating active error minimization. *Physical Review X*, 7(2):021050, 2017.

[McArdle et al.(2019)McArdle, Mayorov, Shan, Benjamin, and Yuan] Sam McArdle, Alexander Mayorov, Xiao Shan, Simon Benjamin, and Xiao Yuan. Digital quantum simulation of molecular vibrations. *Chemical science*, 10(22):5725–5735, 2019.

[McClean et al.(2016)McClean, Romero, Babbush, and Aspuru-Guzik] Jarrod R. McClean, Jonathan Romero, Ryan Babbush, and Alán Aspuru-Guzik. The theory of variational hybrid quantum-classical algorithms. *New Journal of Physics*, 18(2):1–20, 2016. ISSN 13672630. doi: 10.1088/1367-2630/18/2/023023.

[McLachlan(1964)] A. McLachlan. A variational solution of the time-dependent schrodinger equation. *Mol. Phys.*, 8(39–44), 1964.

[Neill Lambert(2013)] Yuan-Chung Cheng Che-Ming Li Guang-Yin Chen Franco Nori Neill Lambert, Yueh-Nan Chen. Quantum biology. *Nature Physics*, 9:10–18, 2013.

[Nobuyuki Yoshioka(2019)] Kousuke Mitarai Keisuke Fujii Nobuyuki Yoshioka, Yuya O. Nakagawa. Variational Quantum Algorithm for Non-equilibrium Steady States. *arXiv preprint*, page arXiv:1908.09836v3, 2019. URL http://https://arxiv.org/abs/1908.09836.
[P. W. Langhoff and Karplus(1972)] S. T. Epstein P. W. Langhoff and M. Karplus. Aspects of time-dependent perturbation theory. *Rev. Mod. Phys.*, 44(602), 1972.

[P.M.A.Dirac(1930)] P.M.A.Dirac. Note on exchange phenomena in the thomas atom. *Proc. Cambridge Philos. Soc.*, 30(376), 1930.

[Shi-Jie Wei(2016)] Gui-Lu Long Shi-Jie Wei, Dong Ruan. Duality quantum algorithm efficiently simulates open quantum systems. *Scientific Reports*, 6(30727), 2016.

[Somma et al.(2003)Somma, Ortiz, Knill, and Gubernatis] Rolando Somma, Gerardo Ortiz, Emanuel Knill, and James Gubernatis. Quantum simulations of physics problems. *International Journal of Quantum Information*, 1(02):189–206, 2003.

[Suzuki(1990)] Masuo Suzuki. Fractal decomposition of exponential operators with applications to many-body theories and monte carlo simulations. *Physics Letters A*, 146(319–323), 1990.

[Suzuki(1991)] Masuo Suzuki. General theory of fractal path integrals with applications to many-body theories and statistical physics. *Journal of Mathematical Physics*, 32(400–407), 1991.

[Zixuan Hu(2020)] Sabre Kais Zixuan Hu, Rongxin Xia. A quantum algorithm for evolving open quantum dynamics on quantum computing devices. *Scientific Reports*, 10(3301), 2020.