


Hermitian-preserving ansatz and variational open quantum eigensolver

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We propose a variational quantum algorithm named variational open quantum eigensolver (VOQE) for solving steady states of open quantum systems described by either Lindblad master equations or non-Hermitian Hamiltonians. In VOQE, density matrices of mixed states are represented by pure states in doubled Hilbert space. We give a framework for building a circuit ansatz which we call the Hermitian-preserving ansatz to restrict the searching space. We also give a method to efficiently measure the operators' expectation values by postselection measurements. We show the workflow of VOQE on solving steady states of the Lindblad master equations of the driven XXZ model and implement VOQE to solve the spectrum of the non-Hermitian Hamiltonians of the Ising spin chain in an imaginary field.

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I. INTRODUCTION

In noisy intermediate-scale quantum (NISQ) devices [1], due to the lack of quantum error correction [2], quantum circuits are shallow and noisy, which limits the implementations of most quantum algorithms [3]. To make NISQ devices useful for practical problems, variational quantum algorithms (VQA) were proposed [4]. The central idea of these algorithms is evaluating quantumly and optimizing classically a cost function whose minimum (or maximum) value corresponds to the problem solution. Due to the low requirements on quantum circuits assisted by quantum error mitigation methods [5], VQAs have become perhaps the most promising application in the NISQ era and have attracted much attention during the past few years.

In this work we focus on utilizing the idea of VQAs to solve problems in an important area of quantum mechanics, the open quantum systems. When a system has interactions with the environment, the behaviors of such a system can be much richer. To describe the dynamics of such systems, mixed-state descriptions, nonunitary transformations, etc. need to be introduced to generalize Schrödinger's equation. Among many formalisms, the Lindblad master equation (LME) [6] and non-Hermitian Hamiltonian (nHH) [7] evolutions are rather popular and have their own successfully applicable scopes. Since the dimension of the Hilbert space can be exponentially large, solving these equations classically can be rather inefficient [6], which leads to the demands on using quantum computers to solve them. There have been several proposals for open quantum systems [8–13]. Here, we present another new variational quantum algorithm, which we call the variational open quantum eigensolver (VOQE), to

solve an important topic: the steady states of open quantum systems. (Hereafter, the steady states correspond to not only those of LMEs but also the right eigenstates of this.) In the following, we will first show the basic theory of VOQE, which can solve the steady states of both the LME and nHH, and then verify the effectiveness of VOQE on concrete problems.

LME is a rigorous quantum description of microscopic open quantum systems assuming the Markov approximation of the environment. An LME can be expressed as

$$\frac{d\rho}{dt} = \mathcal{L}[\rho] = -i[H, \rho] + \sum_i \gamma_i \left(F_i \rho F_i^\dagger - \frac{1}{2} \{ \rho, F_i^\dagger F_i \} \right), \quad (1)$$

where the Hamiltonian H is the unitary part of the dynamics, and F_μ are quantum jump operators with strength γ_μ describing the dissipative channels induced by the environment. For macroscopic scales, we can instead use the nHH, a semi-classical approach to encapsulate behaviors of open quantum systems. The evolution under an nHH, $H_{nh} = H - i\Gamma$, where H and Γ are Hermitian operators, can be described as

$$\frac{d\rho}{dt} = \mathcal{N}[\rho] = -i[H, \rho] - \{\Gamma, \rho\} + 2\text{Tr}(\Gamma\rho)\rho. \quad (2)$$

The last term in Eq. (2) is added to preserve the overall probability, i.e., $\text{Tr}(\rho) = 1$. nHHs have rich properties, such as the PT -symmetry phases and the exceptional points [7], which have attracted much attention in recent years. VOQE aims to solve the steady states of both Eqs. (1) and (2), i.e., $\mathcal{L}[\rho_{lss}] = 0$ and $\mathcal{N}[\rho_{nss}] = 0$. Note that $\mathcal{N}[\rho_{nss}] = 0$ actually is the condition for eigenstates of nHHs. The basic sketch of VOQE is shown in Fig. 1(a). In the following we will explain details of the algorithm, including the cost function, the circuit ansatz, and the way to evaluate operators' expectation values.

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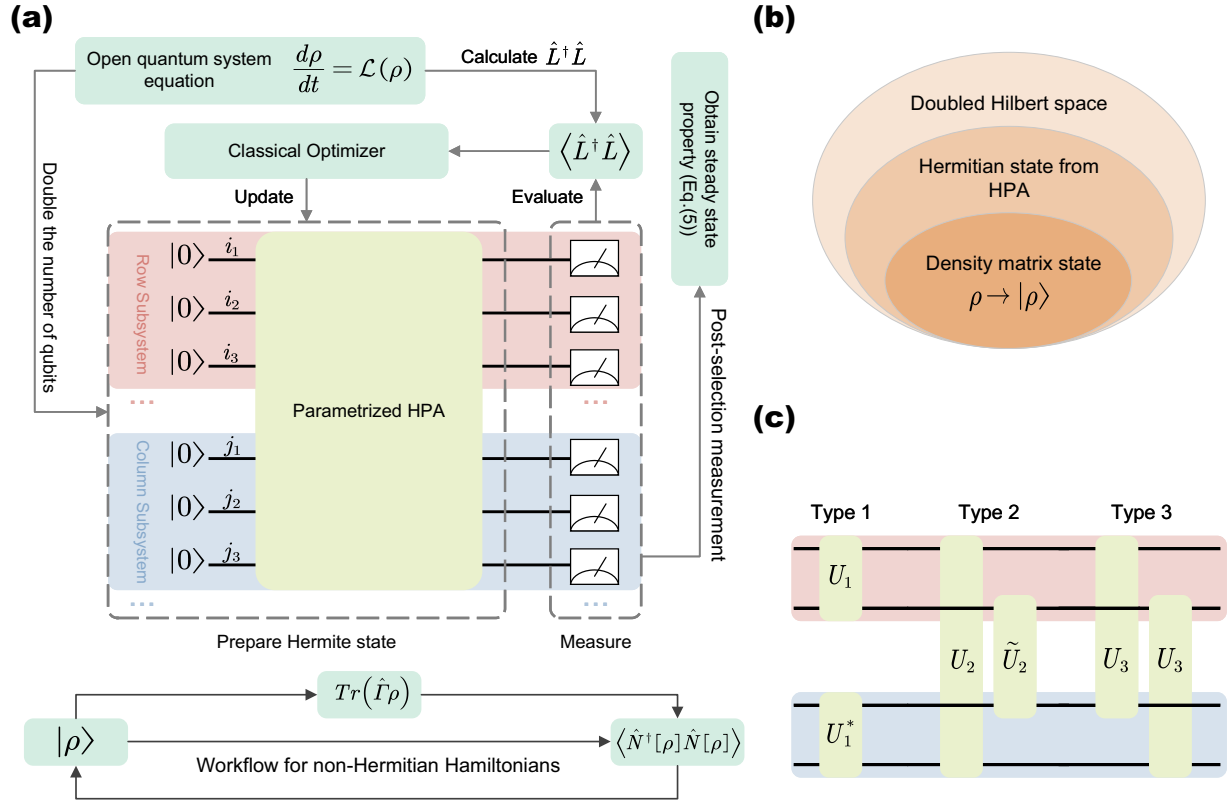


FIG. 1. Variational open quantum eigensolver (VOQE). (a) The sketch of VOQE. VOQE uses $2n$ -qubit (n qubits in row subsystem and n qubits in column subsystem) parameterized HPA to solve the steady state of n -qubit open quantum system equations including LME and nHH. Equations are first transformed into the vector form to obtain the cost function operator. Next, Hermitian states from the conjugate ansatzes are measured to evaluate the cost function value for classical optimization. After the steady state is obtained, a postselection method is used to obtain operators' expectation values of the state. For nHHs, unlike LME, the trace-preserving term in Eq. (2) leads to nonlinear equations, which makes $\text{Tr}[\Gamma\rho]$ appear in $\mathcal{N}[\rho]$. Thus there is an additional intermediate process as shown below. (b) Relations between the whole doubled Hilbert space, Hermitian state space, and density-matrix-state space. Hermitian states have the Hermiticity restriction, while density-matrix states not only require the Hermiticity but also the positive semidefiniteness. (c) Basic HPA blocks. There are three basic blocks when one uses single- or two-qubit gates to compose an HPA. Both types share the idea of pairing to satisfy the HPA conditions Eq. (4). Type 1 describes the unitary transformation process, while type-2 and type-3 simulate the nonunitary process.

II. VOQE

In order to give a measurable cost function for optimizations, we adopt the idea of mapping density matrices to pure states in the doubled Hilbert space $\mathcal{H} \otimes \mathcal{H}$ [8,14]:

$$\rho = \sum_{ij} \rho_{ij} |i\rangle\langle j| \longrightarrow |\rho\rangle = \frac{1}{C} \sum_{ij} \rho_{ij} |i, j\rangle, \quad (3)$$

where $C = \sqrt{\sum_{ij} |\rho_{ij}|^2}$. Note that this encoding is different from the standard purification of mixed states [15] used in many proposals. We call the left subsystem \mathcal{H} of $\mathcal{H} \otimes \mathcal{H}$ the row subsystem (RS) and the right the column subsystem (CS). After this mapping, an operation on the density-matrix $A\rho B$ is transformed into the form $A \otimes B^T |\rho\rangle$. Following this rule, we obtain the vector representation of Eqs. (1) and (2): $\frac{d|\rho\rangle}{dt} = \hat{L}|\rho\rangle$ and $\frac{d|\rho\rangle}{dt} = \hat{N}[\rho]|\rho\rangle$, where \hat{L} and $\hat{N}[\rho]$ are matrices (see Appendix A for concrete forms) acting on $|\rho\rangle$ ($\hat{N}[\rho]$ has dependence on ρ which we will talk about later). The steady state ρ_{ss} will satisfy the condition $C_L[\rho_{ss}] = \langle \rho_{ss} | \hat{L}^\dagger \hat{L} | \rho_{ss} \rangle = 0$ for LME and $C_n[\rho_{ss}] = \langle \rho_{ss} | \hat{N}^\dagger[\rho_{ss}] \hat{N}[\rho_{ss}] | \rho_{ss} \rangle = 0$ for

nHH. Since the Hermitian matrices in this condition have non-negative spectra, we can thus define the cost functions as $C_L[|\rho\rangle]$ and $C_n[|\rho\rangle]$, whose minimum values 0 correspond to steady states [8].

The ansatz circuit in the doubled Hilbert space deserves a careful look. Because density matrices satisfy the Hermiticity and the positive semidefiniteness, pure states mapped from them, which we will call density-matrix states (DMS), only occupy part of the doubled Hilbert space. An ansatz that can only be able to explore DMS has been given in the dissipative-system variational quantum eigensolver (dVQE) [8]. Here, instead, we relax the restriction of the positive semidefiniteness and give another ansatz, which we will call the Hermitian-preserving ansatz (HPA), that can explore states mapped from Hermitian matrices, which we will call Hermitian states satisfying $\langle i, j | \phi \rangle = \langle j, i | \phi \rangle^*$ [Fig. 1(b)]. Since such ansatzes have restricted searching space and are specially designed for open quantum systems, as problem-inspired ansatzes they may have large derivations from a unitary 2 design [4,16] and thus could have less severe barren plateau problems compared with random quantum circuits

[16]. HPA is inspired from the similarity between the Kraus sum representation [6] of general quantum processes and the operator-Schmidt decomposition of unitary operators [17], which has the form

$$U_{\text{HPA}} = \sum_{\alpha} \lambda_{\alpha} A_{\alpha} \otimes A_{\alpha}^*, \quad (4)$$

where λ_{α} are real numbers and A_{α} (A_{α}^*) are orthogonal operators bases in RS (CS), i.e., $\text{tr}[A_{\alpha} A_{\beta}^{\dagger}] = \delta_{\alpha\beta}$. HPA Eq. (4) is actually a representation of orthogonal matrices in real linear space spanned by Hermitian state bases (such as Hermitian states mapped from Pauli operators); thus HPA can preserve Hermitian states and is universal (see proofs in Appendix C). We need to mention that enlarging the searching area will not give wrong answers, i.e., nonphysical steady states (we give a simple proof in the Appendix B).

HPA can be built from three basic types of 2-qubit blocks [Fig. 1(c)]. All three of the blocks share the same idea of pairing gates to satisfy the condition Eq. (4). The first type (type 1) has only one nonzero λ_{α} when written as Eq. (4). This type is simply the tensor product of a unitary operator in RS and its complex conjugate in CS which simulates the unitary transformations of the density matrix. Types 2 and 3 have more than one nonzero λ_{α} which can simulate the nonunitary dissipative transformations of the density matrix and lead to the change of density-matrix eigenvalues. Here, \tilde{U}_2 in type 2 is defined as $\tilde{U}_2 = \sum_{\alpha} \lambda_{\alpha}^* B_{\alpha}^* \otimes A_{\alpha}^*$ acting on qubits i_2 and j_1 in order to make a pair with U_2 expressed as operator-Schmidt $U_2 = \sum_{\alpha} \lambda_{\alpha} A_{\alpha} \otimes B_{\alpha}$ acting on qubits i_1 and j_2 . Due to the pairing, both U_1 and U_2 are arbitrary. For the way of pairing in type 3 (one U_3 acts on qubit i_1 and j_1 while the other acts on qubits 2 and 4), however, the form of U_3 has to be restricted to satisfy Eq. (4). As an example, the CZ gate is a typical type-3 gate that can be U_3 (see details of the three types in the Appendix D).

The last segment of our algorithm uses postselection measurements to obtain the operators' expectation values of steady states. Now suppose we have successfully found the state $|\rho_{ss}\rangle$ corresponding to the steady density matrix ρ_{ss} . The expectation value of an operator O for ρ_{ss} is $\text{Tr}[O\rho_{ss}]$, which can be expressed in terms of $|\rho_{ss}\rangle$:

$$\text{tr}[O\rho_{ss}] = \sum_i \langle i, i | O | \rho_{ss} \rangle / \sum_i \langle i, i | \rho_{ss} \rangle. \quad (5)$$

To measure the right-hand side of Eq. (5), one needs to first rotate $|\rho_{ss}\rangle$ to the eigenvector basis of O and then postselect the measurement samples on all $|i, i\rangle$ bases which correspond to diagonal bases of the density matrix. Suppose after measurements there are m_i samples on the $|i, i\rangle$ basis. Then the right-hand side of Eq. (5) can be estimated by

$$\frac{\sum_i \sqrt{m_i} o_i}{\sum_i \sqrt{m_i}}, \quad (6)$$

where o_i is O 's element at the $|i\rangle\langle i|$ basis. Equation (6) is reasonable because the physical steady solution $|\rho_{ss}\rangle$ has real and positive amplitudes on $|i, i\rangle$ bases. We proved the number of required measurements to achieve an accuracy ε is of order $O(\eta^{-1}\varepsilon^{-4})$, where η is the probability ratio between diagonal and nondiagonal elements of steady states. The ratio η can vary from an exponentially small value (2^{-n} when the density

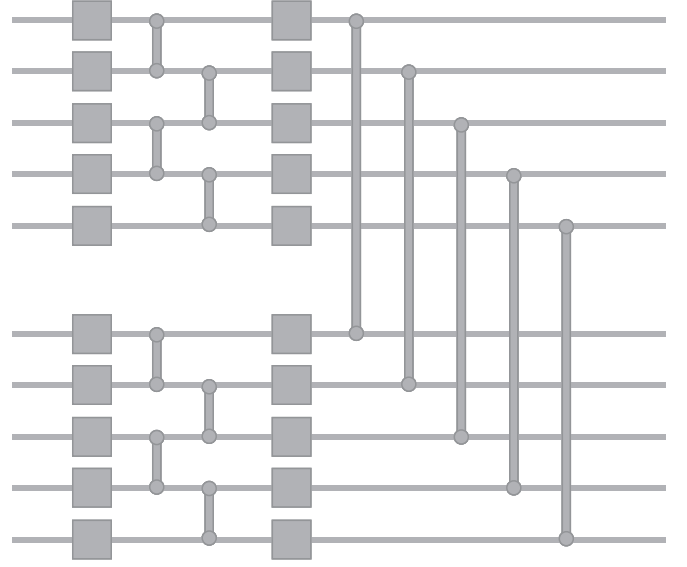


FIG. 2. A layer of the parameterized HPA for the numerical experiments on the driven open XXZ model. During the experiments, we fixed the layer depth to be 1 with additional single-qubit parameterized gates appended at the end of the ansatz. Here, depth means the number of HPA layers shown in this figure.

matrix corresponds to $|+\rangle^{\otimes n}$) to 1 for the maximally mixed state. Roughly speaking, a small purity will lead to a higher η and thus a smaller sampling cost. Thus, this ratio is acceptable for most problem models due to their dissipative nature. (See details about this method and its measurement cost in Appendix E). Note that one can also use Hadamard tests [18] and SWAP tests [19] for evaluating Eq. (5), which however, might be unfriendly for NISQ devices.

These three segments compose the whole structure of VOQE as shown in Fig. 1(a). In general, for an n -qubit open quantum equation, we can build a parameterized $2n$ -qubit HPA to train the steady states and use the measurement protocol to obtain steady-state information. One thing to mention here is that for nHHs, unlike LME, the trace-preserving term in Eq. (2) leads to nonlinear equations, which makes $\text{Tr}[\Gamma\rho]$ appear in $\mathcal{N}[\rho]$. Thus, there is an additional intermediate process for evaluating $\text{Tr}(\Gamma\rho)$. Also, since only type-1 circuits are needed because nHHs will not lead to mixed states, an n -qubit system that prepares trial states $|\psi\rangle$ and $|\psi^*\rangle$ at different times is enough for getting the cost functions.

III. NUMERICAL EXPERIMENTS

To verify the effectiveness of VOQE, we run numerical experiments for specific problems. One is the LME of the driven open XXZ model [20] with the Hamiltonian $H = \sum_i \Delta \sigma_i^z \sigma_{i+1}^z + 2\sigma_i^+ \sigma_{i+1}^- + 2\sigma_i^- \sigma_{i+1}^+$ of open boundaries and two jump channels $F_1 = \sigma_1^+$ and $F_2 = \sigma_n^-$ of strength ϵ . The parameterized circuit for training is composed of type-1 and type-3 gates as shown in Fig. 2. Type-1 gates contain layered single-qubit parameterized gates with the form $e^{-i\theta_x X} e^{-i\theta_y Y} e^{-i\theta_z Z}$ and fixed CZ gates. Note that a single-qubit gate with parameters $\{\theta_x, \theta_y, \theta_z\}$ in RS is paired with a single-qubit gate in the CS with parameters $\{-\theta_x, \theta_y, -\theta_z\}$ to satisfy

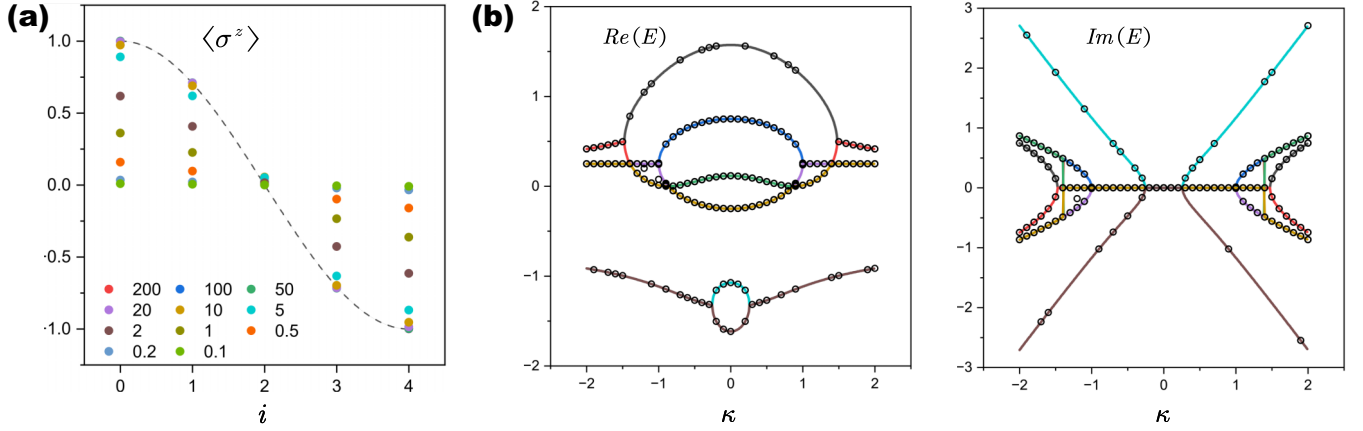


FIG. 3. Numerical experiments of VOQE. (a) The steady states of the LME of the driven open XXZ model. We set $\Delta = 1$ and turn ϵ from 200 to 0.1. There will appear a cosine spin profile $\langle \sigma_i^z \rangle = \cos(\pi \frac{i-1}{n-1})$ as the ϵ increases to a large value. The problem size is 5-qubit, and a 10-qubit HPA is used for training. (b) The complex spectrum of the nHH of the Ising spin chain in an imaginary field. The real part and the imaginary part are plotted, respectively. The solid lines form the exact complex spectrum, and the points are obtained from VOQE. We set $\lambda = 0.5$ and turn κ from -2 to 2 , the spectrums of the Hamiltonians of the model are complex except for the PT -symmetry phases. For each (λ, κ) setting, we run VOQE 30 times to make sure the majority of the spectrum is covered. The problem size is 3-qubit.

the HPA condition. Type-3 gates are CZ gates. For the steady states of this model in the isotropic case $\Delta = 1$, there will appear cosine spin profiles $\langle \sigma_i^z \rangle = \cos(\pi \frac{i-1}{n-1})$ as the ϵ increases to a large value. By turning ϵ from 200 to 0.1, we observe such behaviors in our experiment by variationally preparing the steady states and using Eq. (5) to obtain the spin expectation values of interest. The results can be found in Fig. 3(a). (The convergence of the cost functions with respect to iteration steps can be found in the Appendix F.) The other problem is the nHH of the Ising spin chain in an imaginary field $H = -\frac{1}{2} \sum_i (\sigma_i^z + \lambda \sigma_i^x \sigma_{i+1}^x + i \kappa \sigma_i^x)$ with periodic boundary [21]. The parameterized circuit is composed of only two-qubit gates from type 1 (with a depth of three ignoring type-3 CZ gates in Fig. 2), since nHHs will not lead to mixed states. Since all eigenstates satisfy $C_n[|\rho\rangle] = 0$, we can use the algorithm to draw the spectrum of nHHs by repeated experiments. We set $\lambda = 0.5$ and turn κ from -2 to 2 , and the spectrums of the Hamiltonians of the model are complex except for the PT -symmetry phases. We recover the spectrums in Fig. 3(b). Note that if one wants to find specific eigenstates, penalty terms and preoptimizations [11] can be added. The classical optimization method used throughout the experiments is the Broyden-Fletcher-Goldfarb-Shannon (BFGS) algorithm, assisted by the idea of adiabatic variational optimizing [22,23], where the approximated ground state optimized at a point is chosen as the initial state of points close to it.

IV. COMPARISON WITH RELATED WORKS

Now we want to give a discussion on the comparison between VOQE and other variational quantum algorithms for open quantum systems in Refs. [8–13]. First of all, to the best of our knowledge, compared with these mentioned works, VOQE is the first variational quantum algorithm that can solve steady-state problems of both LME and nHHs in a unified framework. The algorithm proposed in Ref. [9,13] focuses on the variational simulations of dynamics of open quantum systems rather than the steady-state problems. Also, the way

they encode density matrices is by purification [15] rather than vectorization used in VOQE. In Ref. [10], while the authors propose a VQA for the steady states of LME, the purification encoding makes them have to introduce SWAP tests [24] to evaluate a nonlinear cost function. In contrast, by using the vectorization encoding, Ref. [8] and our work are able to use the expectation values of $L^\dagger L$ as natural cost functions that can be easily evaluated by the direct operator averaging method [25]. Compared with Ref. [8], HEA proposed in VOQE can have a more flexible structure and thus has potentially better friendliness for NISQ hardware. Also, we gave an alternative measurement strategy for obtaining steady-state information. References [11,12] focus on using the variational framework to solve nHH problems. In Ref. [11], the authors use the variances of nHH energy as the cost functions and cannot be directly generalized to LME. In Ref. [12] the authors gave a variational quantum algorithm for the eigenvalues of nHHs based on diagonalizations, which require complicated quantum circuits that are unfriendly for NISQ devices.

V. SUMMARY AND OUTLOOK

In summary, we have presented a variational quantum algorithm for solving the steady states of LMEs and nHHs. Density matrices are mapped to pure states in the doubled Hilbert space for measurable cost functions. We constructed the Hermitian-preserving ansatz to restrict the searching space. We want to mention that the applications of such Hermitian-preserving ansatzes should not be restricted to VOQE and can be further investigated. We also gave a postselection measurement method to evaluate operators' expectation values of the steady states. Our algorithms are tested for specific problems, and the results coincide with the theoretical predictions. We hope this work will show a future application for NISQ devices and motivate people to utilize the idea of variational quantum algorithms for solving various problems.

We used the Qulacs [26] for our numerical experiments.

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APPENDIX A: CONCRETE FORMS OF \hat{L} AND $\hat{N}[\rho]$

$$\hat{L} = (-i(H \otimes I - I \otimes H^T) + \sum_i D[\Gamma_i])$$

$$\text{where } D[\Gamma_i] = F_i \otimes F_i^* - \frac{1}{2} F_i^\dagger F_i \otimes I - I \otimes \frac{1}{2} F_i^T F_i^*, \quad (\text{A1})$$

$$\hat{N}[\rho] = -i(H \otimes I - I \otimes H^T) - (\Gamma \otimes I + I \otimes \Gamma^T) + 2\text{Tr}[\Gamma\rho]I \otimes I. \quad (\text{A2})$$

APPENDIX B: UNIQUENESS OF $|\rho_{ss}\rangle$

We assume the condition is there is only one unique steady density matrix of a LME. However, the question is if the uniqueness will still hold if we enlarge the density-matrix states to the Hermitian states, since there may exist other non-density-matrix states that are eigenvectors of the Liouvillian operator \hat{L} of the LME with zero eigenvalues.

Suppose there is not only one unique steady density-matrix state $|\rho_{ss}\rangle$ but also one Hermitian steady state $|\rho_h\rangle$. We can decompose $|\rho_h\rangle$ into

$$|\rho_h\rangle = c_1|\rho_1\rangle + c_2|\rho_2\rangle, \quad (\text{B1})$$

where c_1 and c_2 are real numbers, and $|\rho_1\rangle$ and $|\rho_2\rangle$ are the density-matrix state. $|\rho_1\rangle$ and $|\rho_2\rangle$ can further be decomposed as

$$|\rho_1\rangle = |\rho_{ss}\rangle + |\rho'_1\rangle, \quad |\rho_2\rangle = |\rho_{ss}\rangle + |\rho'_2\rangle. \quad (\text{B2})$$

Thus, we have

$$|\rho_h\rangle = (c_1 + c_2)|\rho_{ss}\rangle + c_1|\rho'_1\rangle + c_2|\rho'_2\rangle. \quad (\text{B3})$$

Due to the unique steady density-matrix-state condition, $|\rho'_1\rangle$ and $|\rho'_2\rangle$ must be linear combinations of eigenvectors of the Liouvillian operator \hat{L} of a LME with nonzero eigenvalues. Therefore, $|\rho_h\rangle$ cannot be a steady Hermitian state, which proves VOQE will not give a wrong answer. nHH will not have this issue, since only type-1 circuits are required.

APPENDIX C: HPA

A completely positive transformation (CPT) can be written as the Kraus sum

$$\rho \rightarrow \sum_{\alpha} M_{\alpha} \rho M_{\alpha}^{\dagger}. \quad (\text{C1})$$

If we only want to keep Hermiticity of the matrix, Eq. (C1) can be adjusted to

$$\rho \rightarrow \sum_{\alpha} \eta_{\alpha} M_{\alpha} \rho M_{\alpha}^{\dagger}, \quad (\text{C2})$$

where η_{μ} is real. To keep the trace of the matrix 1, the following equation must be obeyed:

$$\sum_{\alpha} \eta_{\alpha} M_{\alpha}^{\dagger} M_{\alpha} = I. \quad (\text{C3})$$

However, in order to keep an HPA described as

$$U_{\text{HPA}} = \sum_{\alpha} \lambda_{\alpha} A_{\alpha} \otimes A_{\alpha}^*, \quad (\text{C4})$$

to be unitary, it must obey

$$\sum_{\alpha\beta} \lambda_{\alpha} \lambda_{\beta} A_{\alpha}^{\dagger} A_{\beta} \otimes A_{\alpha}^T A_{\beta}^* = I. \quad (\text{C5})$$

Equations (C3) and (C5) are the same condition if and only if the HPA is composed of only type-1 circuit blocks. For other types, HPA and Kraus sums are not one-to-one correspondence.

A universal HPA form of Eq. (C4) can be obtained by considering orthogonal matrices of linear space spanned by Hermitian state bases. An orthogonal matrix U_{HPA} in this space can be expressed as diagonal form,

$$U_{\text{HPA}} = \sum_{\beta} \zeta_{\beta} |\Psi^{\beta}\rangle \langle \Psi^{\beta}|, \quad (\text{C6})$$

where $\zeta_{\beta} = \pm 1$ and $|\Psi^{\beta}\rangle = \sum_{ij} \Psi_{ij}^{\beta} |i, j\rangle$ satisfy the Hermitian state condition $\Psi_{ij}^{\beta} = \Psi_{ji}^{\beta*}$. The elements of the HPA satisfy

$$\begin{aligned} M_{ik,jl} &= \langle i, j | U_{\text{HPA}} | k, l \rangle = \sum_{\beta} \zeta_{\beta} \Psi_{ij}^{\beta} \Psi_{kl}^{\beta*} = \sum_{\beta} \zeta_{\beta} (\Psi_{ji}^{\beta} \Psi_{lk}^{\beta*})^* \\ &= \langle j, i | U_{\text{HPA}} | l, k \rangle^* = M_{jl,ik}^* \end{aligned}$$

Equation (C7) is the necessary and sufficient condition of a unitary operator to be an HPA. We see M is a Hermitian matrix (by treating ik as row index and jl as column index). By diagonalizing M , we have $M = T \lambda T^{\dagger}$, where T is unitary and λ is diagonal with real diagonal entries λ_{α} . Now we can express Eq. (C6) as

$$\begin{aligned} U_{\text{HPA}} &= \sum_{ijkl} M_{ik,jl} |i, j\rangle \langle k, l| = \sum_{ijkl\alpha} T_{ik\alpha} \lambda_{\alpha} T_{\alpha jl}^{\dagger} |i\rangle \langle k| \otimes |j\rangle \langle l| \\ &= \sum_{\alpha} \lambda_{\alpha} \left(\sum_{ik} T_{ik\alpha} |i\rangle \langle k| \right) \otimes \left(\sum_{jl} T_{jl\alpha}^* |j\rangle \langle l| \right) \\ &= \sum_{\alpha} \lambda_{\alpha} A_{\alpha} \otimes A_{\alpha}^*. \end{aligned} \quad (\text{C7})$$

It is easy to check that $A_{\alpha} = \sum_{ik} T_{ik\alpha}$ are orthonormal operator bases; thus we have proved Eq. (C4). The proof process is similar to the operator-Schmidt decomposition [17], where single-value decomposition (SVD) replaces the diagonalization process.

APPENDIX D: HPA TYPES

The first type of Eq. (C4) corresponds to only one nonzero λ_α . This type is simply the tensor product of a unitary operator U_1 in RS and its complex conjugate in CS, which simulates the unitary transformation of the density matrix:

$$U_{T1} = U_1 \otimes U_1^*. \quad (\text{D1})$$

For the second type, it is easy to check

$$U_{T2} = U_2 \otimes \tilde{U}_2 = \sum_{\alpha\beta} \lambda_\alpha \lambda_\beta (A_\alpha \otimes B_\beta^*) \otimes (A_\beta^* \otimes B_\alpha), \quad (\text{D2})$$

and one can further prove

$$\begin{aligned} \langle i, j | U_{T2} | k, l \rangle &= \sum_{\alpha\beta} \lambda_\alpha \lambda_\beta (A_\alpha \otimes B_\beta^*)_{ik} \otimes (A_\beta^* \otimes B_\alpha)_{jl} \\ &= \sum_{\alpha\beta} \lambda_\alpha \lambda_\beta (A_\alpha \otimes B_\beta^*)_{ik} (A_\beta^* \otimes B_\alpha)_{jl} \\ &= \sum_{\alpha\beta} \lambda_\alpha \lambda_\beta (A_\beta \otimes B_\alpha^*)_{jl}^* (A_\alpha^* \otimes B_\beta)_{ik}^* \\ &= \sum_{\beta\alpha} \lambda_\beta \lambda_\alpha (A_\beta \otimes B_\alpha^*)_{jl}^* (A_\alpha^* \otimes B_\beta)_{ik}^* \\ &= \langle j, i | U_{T2} | l, k \rangle^*, \end{aligned} \quad (\text{D3})$$

which exactly satisfies the condition Eq. (C7). Thus U_{T2} is an HPA block.

The U_3 in type 3 has restricted form, which can be directly obtained from Eq. (C7):

$$\begin{bmatrix} M_{0000} & M_{0001} & M_{0001}^* & M_{0101} \\ M_{0010} & M_{0011} & M_{0110} & M_{0111} \\ M_{0010}^* & M_{0110}^* & M_{0011}^* & M_{0111}^* \\ M_{1010} & M_{1011} & M_{1011}^* & M_{1111} \end{bmatrix}, \quad (\text{D4})$$

from which one can obtain the type 3:

$$U_{T3} = U_3 \otimes U_3. \quad (\text{D5})$$

Thus, U_3 does not need a pairing procedure, since U_3 itself has satisfied the condition.

APPENDIX E: POSTSELECTION MEASUREMENT

In this Appendix we show how to evaluate Eq. (5) by measurements and give the measurement cost of it. We first assume that O is diagonal in the $|i\rangle$ basis, i.e., $O_{ij} = o_i \delta_{ij}$. Then Eq. (5) can be rewritten as

$$\begin{aligned} & \sum_i \langle i, i | O \otimes I | \rho_{ss} \rangle / \sum_i \langle i, i | \rho_{ss} \rangle \\ &= \sum_{ikl} \rho'_{sskl} \langle i | O | k \rangle \delta_{il} / \sum_i \rho'_{ssii} \\ &= \sum_{ikl} \rho'_{sskl} o_i \delta_{ik} \delta_{il} / \sum_i \rho'_{ssii} \\ &= \sum_i \rho'_{ssii} o_i / \sum_i \rho'_{ssii}. \end{aligned} \quad (\text{E1})$$

$\rho'_{ssii} = \rho_{ssii}/C$ are real and non-negative because the steady state corresponds to a physical density matrix, which means it can be evaluated by measurements. Consider that we repeat the measurements for totally M times. If m_i samples are obtained on the $|i, i\rangle$ basis and $\sum_i m_i = m$, then the postselection efficiency is $\eta = \frac{m}{M}$, which depends on the probability ratio between diagonal and nondiagonal elements of steady states. For many dissipation models, nondiagonal elements decay to near zero, and thus η are acceptable. Equation (E1) can be evaluated by postselection and postprocessing:

$$\sum_i \rho'_{ssii} o_i \approx \frac{\sum_i \sqrt{\frac{m_i}{m}} o_i}{\sum_i \sqrt{\frac{m_i}{m}}} = \frac{\sum_i \sqrt{m_i} o_i}{\sum_i \sqrt{m_i}}. \quad (\text{E2})$$

The variance of the right-hand side of Eq. (E2) is

$$\text{Var} \left[\frac{\sum_i \sqrt{m_i} o_i}{\sum_i \sqrt{m_i}} \right] = \frac{\text{Var}[O]}{\sum_i \sqrt{m_i}} \leq \frac{\text{Var}[O]}{\sqrt{m}} = \frac{\text{Var}[O]}{\sqrt{\eta M}}. \quad (\text{E3})$$

Thus the measurement cost we need to achieve a variance of ϵ^2 in the worst case is

$$M(\epsilon) \approx \frac{1}{\eta} \left(\frac{\text{Var}[O]}{\epsilon^2} \right)^2. \quad (\text{E4})$$

For general O , we need to decompose them on different measurement bases (Pauli bases) $O = \sum_{\gamma=1}^K O_\gamma$ to evaluate the expectation value of each part individually, as discussed in Ref. [25], and a similar result can be obtained,

$$M(\epsilon) \approx K \left(\frac{\sum_\gamma \text{Var}[O_\gamma] / \sqrt{\eta_\gamma}}{\epsilon^2} \right)^2, \quad (\text{E5})$$

where η_γ is the efficiency of the steady state in the diagonal basis of O_γ .

APPENDIX F: CONVERGENCE OF COST FUNCTIONS IN NUMERICAL EXPERIMENTS

In this appendix, we show the convergence of cost functions under random initial parameters (Fig. 4).

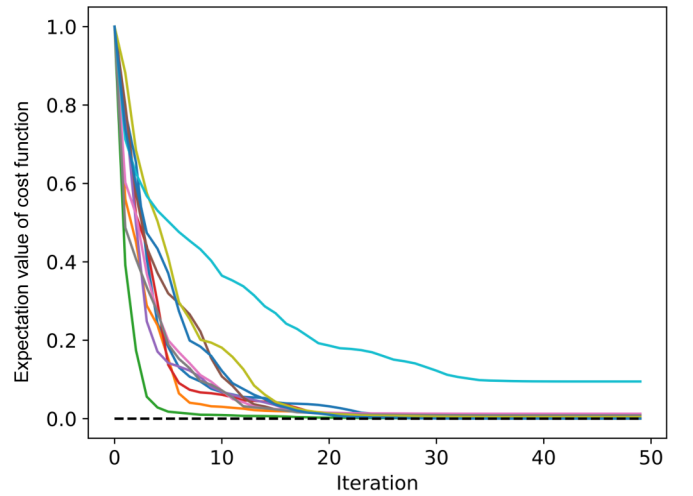


FIG. 4. Convergence of the cost functions of the driven open XXZ model with $\epsilon = 1$ under random initialization as functions of iteration steps. For each cost function, we have rescaled its range within $[0,1]$ to have a better presentation. The starting point (initial parameters) of each curve is chosen randomly. The optimizer is chosen to be the BFGS optimizer.

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