Convex Optimization for Nonequilibrium Steady States on a Hybrid Quantum Processor

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Finding the transient and steady state properties of open quantum systems is a central problem in various fields of quantum technologies. Here, we present a quantum-assisted algorithm to determine the steady states of open system dynamics. By reformulating the problem of finding the fixed point of Lindblad dynamics as a feasibility semidefinite program, we bypass several well-known issues with variational quantum approaches to solving for steady states. We demonstrate that our hybrid approach allows us to estimate the steady states of higher dimensional open quantum systems and discuss how our method can find multiple steady states for systems with symmetries.

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Introduction.—Understanding open system evolution is central to modern quantum technologies such as computing, thermodynamics [1–3], chemistry [4], and quantum transport [5]. Since such evolution maps initial quantum states to future states, both transient and steady state properties are available in the structure of the evolution operator. Sparing few analytically tractable systems, generic open system evolution has to be solved numerically to understand both transient and steady state dynamics of the system. Such classical simulation techniques are limited due to the exponential growth of Hilbert space. Some specific sampling problems can be simulated classically [6–9] and tensor networks can be deployed for scenarios with limited entanglement growth [10–17]. For generic open system evolution by contrast, such a classical simulation is limited to few dozen qubits in the presence of symmetries. Usually, such problems are either simplified by the presence of strong local dissipators which reduce the amount of entanglement generated or by low dimensionality of the problem. Outside of these special cases, the issue of generic open system evolution has remained unsolved.

The advent of small quantum computers heralds a new variety of solutions to the problem of determining the transient and steady state solutions to such open system evolution. One strategy involves implementing open system evolution on an intermediate scale quantum computer and tomographically measuring the quantum state at various times [18]. An equivalent method for completely positive maps would be to quantum simulate and measure the Choi matrix associated with the open system evolution [19–21]. These tomographic methods require exponentially large number of measurements and hence are practically infeasible. Another group of closely related strategies involves first implementing $\mathcal{L}$, the Liouville superoperator associated with the open system evolution, on a quantum computer. After implementing $\mathcal{L}$ on a quantum computer, the different strategies to find the nonequilibrium steady states (NESSs) include methods like a combination of Trotterization and imaginary time evolution using $\mathcal{L}$ [22], quantum phase estimation on $\mathcal{L}$ [23], and variational quantum algorithms (VQAs) to find the kernel of $\mathcal{L}^\dagger\mathcal{L}$ [24]. These different but related strategies have their own individual drawbacks. Trotterization and phase estimation approaches are known to be infeasible on our current quantum devices with short coherence times, and the variational optimization approaches suffer from the difficulty of optimizing over a nonconvex space [25–27]. Lastly, all of these methods that rely on the superoperator representation $\mathcal{L}$ of the open system evolution suffer from the large dimensionality of the Liouville space.

In this Letter, we propose a hybrid algorithm for the determination of NESSs. Through our approach, the steady state problem can be recast as solving a feasibility

semidefinite program (SDP) [28–30]. We show that such an approach to find the NESS is viable on a near-term intermediate scale quantum (NISQ) device. Our first contribution is to restate the NESS problem as a feasibility SDP, which is a SDP where the goal is to find a feasible solution satisfying the positive semidefinite and linear constraints [28–30]. Our second contribution is that we do not use a variational quantum state or circuit as the *Ansatz* [24,31–33]. By doing so, we bypass the problems [34–37] associated with training variational quantum algorithms with their nonconvex landscape, which is known to be nondeterministic polynomial-time (NP) hard [25–27]. We show that our algorithm naturally enforces positivity constraint of a physical density matrix and provides methods to enforce additional constraints systematically while retaining the advantages of quantum-assisted methods [35,37–40], like providing a method to systematically gain a more expressible, problem-aware *Ansatz*.

Nonequilibrium steady states.—Open system dynamics under Born, Markov and secular approximations are often described by a time-local master equation given by $\dot{\rho} = L[\rho]$, where

$$L[\rho] = -i[H,\rho] + \sum_n \gamma_n \left(A_n \rho A_n^\dagger - \frac{1}{2}\{A_n^\dagger A_n, \rho\} \right).$$

Such an evolution preserves conditions for valid density matrices. The transient and steady states of this evolution are characterized by the spectrum of the Liouville superoperator [5], defined by the vectorization $B\rho C \to C^* \otimes B|\rho\rangle$. Steady states are understood to satisfy $L[\rho] = 0$ or equivalently $\mathcal{L}|\rho\rangle = 0$, where $\mathcal{L}$ is the Liouville superoperator that arises from the vectorization of L. Since these steady states do not usually correspond to a thermal equilibrium, they are referred to as nonequilibrium steady states. We refer to the problem of obtaining the steady state(s) of a given Liouville evolution as the NESS problem, which is solved classically by matrix diagonalization. However, due to the increase in dimensionality, diagonalization of the full spectrum is usually unfeasible. Furthermore, the evolution of n-dimensional density matrices in Liouville space are represented by $n^2 \times n^2$ matrices. This squared dimensionality implies that numerical techniques can find the entire spectrum of only modest open quantum systems, usually relying on Arnoldi-type methods [41–44], which become quite cumbersome for many-body systems of moderate size.

Hence, there is interest in understanding if quantum computers, with their inherent dimensionality advantages in simulating quantum systems over classical computers, can solve the NESS problem. For NISQ devices, it was shown that the NESS problem can be mapped to a variational problem in Liouville space [24]. The subsequent variational problem is solved by using a parametrized quantum state or quantum circuit as the *Ansatz*, and relies on forms of VQA. This approach has two main concerns. Firstly, it is unclear how to systematically enforce the positivity constraint for the density matrix in this approach, as the variational quantum state or quantum circuit, which is a vector, must eventually correspond to a physical density matrix using the vectorization described above. Secondly, optimizing over the set of pure states tends to not be convex and hence difficult, and indeed has been shown to be NP-hard, reasons including the parameter landscape containing exponentially many persistent local minima that are far from the global minimum [25–27] (see Supplemental Material [45]). Other VQA methods that do not explicitly rely on this map to Liouville space [31] face similar problems.

Quantum feasibility SDP approach.—We circumvent the nonconvex optimization problem in the Liouville space by optimizing over the convex set of density matrices. This allows us to directly apply a feasibility SDP, one consequence of which is that we can now systematically enforce the positive semidefinite condition. A feasibility SDP admits the following form: Find $X, X \in S_+^l$ such that $\mathrm{Tr}(C_k X) = v_k,\ \forall\ k \in 1, 2, \ldots, c$. Here, $\mathcal{S}_+^l$ represents the set of $l \times l$ symmetric positive semidefinite (PSD) matrices. This is the problem of determining if it is possible to find a matrix X subject to the PSD constraint and the other given constraints. The matrices C_k belong to the set of symmetric matrices $\mathcal{S}^l$ for $k \in \{1, 2, \ldots, c\}$. The kth element of vector $v \in \mathbb{R}^c$ is denoted by v_k. SDPs can be formulated for complex-valued matrices via a cone of Hermitian positive semidefinite matrices, i.e., $X \in \mathcal{H}_+^l$. Since SDPs for real-valued matrices are a special case of SDPs for complex-valued matrices, we will consider the latter case in this Letter. Since $\dot{\rho} = L[\rho]$ is linear in ρ, the NESS problem is a feasibility SDP.

We consider a state *Ansatz* of the form

$$\rho = \sum_{i,j} \beta_{ij} |\chi_i\rangle\langle\chi_j|. \tag{1}$$

Here, β_{ij} are matrix elements of a positive semidefinite matrix β, whereas $|\chi_i\rangle$ states can be from any set of quantum states. We see that β being positive semidefinite is both a necessary and sufficient condition for ρ to be positive semidefinite. The condition $\mathrm{Tr}(\rho) = 1$ becomes $\mathrm{Tr}(\beta E) = 1$, where E is a matrix with matrix elements $E_{ij} = \langle\chi_i|\chi_j\rangle$.

With the chosen *Ansatz*, the NESS problem becomes

$$\text{find}\, \beta \,\text{such that}\ -i(D\beta E - E\beta D) + \sum_n \gamma_n \left(R_n \beta R_n^\dagger - \frac{1}{2} F_n \beta E - \frac{1}{2} E \beta F_n \right) = 0, \tag{2}$$

$$\beta \succeq 0, \tag{3}$$

$$\mathrm{Tr}(\beta E) = 1, \tag{4}$$

where γ_n are the strengths of the dissipators, D, R, F are matrices defined as $D_{ij} = \langle\chi_i|H|\chi_j\rangle$, $(R_n)_{ij} = \langle\chi_i|A_n|\chi_j\rangle$, and $(F_n)_{ij} = \langle\chi_i|A_n^\dagger A_n|\chi_j\rangle$. This reduction of the NESS problem to a feasibility SDP [29,68] defined over β is motivated by the idea that a judicious choice of the states $|\chi_i\rangle$ in some problem-aware manner could possibly allow us to do an optimization over a smaller dimensional convex landscape (compared to ρ). Furthermore, the positive semidefiniteness condition of ρ can be enforced naturally. We utilize CVX [69], which relies on a disciplined convex programming algorithm [70,71].

We can also easily enforce additional linear constraints of the form $\mathrm{Tr}(\beta X) = x$, where X and x are arbitrary matrices and values, respectively. This feature of our scheme is absent in the existing algorithms for solving NESSs on NISQ devices and is further discussed below.

The overlap values for the matrix elements of the E, D, R, F matrices can be measured on a NISQ quantum computer [72]. In general, how we choose the $|\chi_i\rangle$ states to form our *Ansatz* will contribute strongly to how our algorithm scales. For a general Hamiltonian, absent of exploitable symmetries, the size of the optimal *Ansatz* will grow exponentially with the size of the problem. (see Supplemental Material [45]). Even in the worst case where we require exponentially large numbers of $|\chi_i\rangle$ states in our *Ansatz*, we do not map the problem to an equivalent one in Liouville space and avoid the aforementioned squared dimensionality that comes from doing optimization in Liouville space. Hence in the worst case, our method is at least quadratically better than analogous variational algorithms.

Unless otherwise stated, we choose cumulative $\mathcal{K}$ moment states ($\mathbb{CS}_K$ states) [39] which provide us with a systematic way to generate an increasingly expressible problem-aware *Ansatz*. These states rely heavily on calculating expectation values of powers of the Hamiltonian $\langle\psi|H^k|\psi\rangle$ which can be done efficiently [73,74]. They alternatively can also be easily obtained by calculating the expectation value of Pauli strings [38,39] (see Ref. [45] for details). By using the $\mathbb{CS}_K$ states as an *Ansatz*, the size of the β matrix that will be calculated scales as δ^K, where δ is the number of terms in the Hamiltonian, for small K. While this is typically not scalable, we emphasize that our method need not use $\mathbb{CS}_K$ states as its *Ansatz*. Our main contribution is in approaching the steady state problem in terms of a SDP, and the choice of *Ansatz* in our Letter is secondary. A more efficient method of generating an *Ansatz* can be used, if we have greater knowledge of the underlying symmetries of the system. Note that the SDP itself could also be sped up with the help of a quantum computer [75].

The algorithm can hence be summarized as (a) choose a hybrid *Ansatz* for ρ using a set of chosen quantum states $\{|\chi_i\rangle\}$, (b) calculate the entries of the overlap matrices on the quantum computer, (c) use the matrices in a SDP optimization routine run on a classical computer to obtain the approximate NESS.

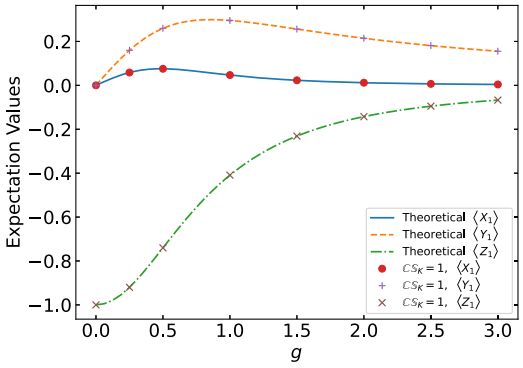

FIG. 1. Expectation values for 2-qubit transverse field Ising model. γ's set at 1. Fidelity is equal to 1 for all values of g. Our method gives strong agreement with the theoretical results.

Examples.—We demonstrate our algorithm with some examples. Consider a 2-qubit transverse field Ising model with the Hamiltonian $H_2 = (1/2)\sigma_Z^1\sigma_Z^2 + g\sigma_X^1 + g\sigma_X^2$, together with local dissipators $A_1 = \sigma_Z^1$, $A_2 = (1/2)(\sigma_X^1 - i\sigma_Y^1)$, $A_3 = \sigma_Z^2$, and $A_4 = (1/2)(\sigma_X^2 - i\sigma_Y^2)$. For all instances presented in Fig. 1, our hybrid algorithm outputs a density matrix ρ that is unit trace, Hermitian, positive semidefinite, and that fulfills the NESS condition $\dot{\rho} = 0$. To study the robustness of the algorithm for larger chains, in Fig. 2 we show simulation results for the transverse field Ising model up to 8 qubits. For the 5-qubit and 8-qubit systems presented in Fig. 2, when increasing K, we choose from the $\mathbb{CS}_K$ *Ansatz*, a random subset of new states, as highlighted in the Supplemental Material [45]. A comparison with the existing NISQ approach in Ref. [24] for the 8-qubit case is also given in the Supplemental Material [45].

We note that for the model chosen, as g increases, the exact NESS solution has larger rank and is less sparse. We find that for such situations, a larger *Ansatz* size is needed to obtain an approximate NESS with similar fidelity. We also note that the $\mathbb{CS}_K$ *Ansatz* performs efficiently when the steady states are low rank. When this is not the case, it is expected that any NISQ algorithm based on such *Ansätze* will underperform. Likewise, we note that another choice that significantly influences the *Ansatz* is the choice of initial states, where recent results on solving the ground state problem can aid in providing useful initial states [76].

Strong symmetries.—One additional complication with the NESS problem is that systems with symmetries can exhibit multiple NESSs [5]. Our algorithm can also be extended to certain cases where multiple NESSs are expected. If there is a strong symmetry in the system, then the Hilbert space can be decomposed into the symmetry subspaces, namely,

$$\mathcal{H} = \bigoplus_{\alpha=1}^{n_U} \mathcal{H}_\alpha, \qquad \mathcal{H}_\alpha = \mathrm{Span}\{|\psi_\alpha^{(k)}\rangle\}, \qquad k \in [1, d_\alpha]. \tag{5}$$

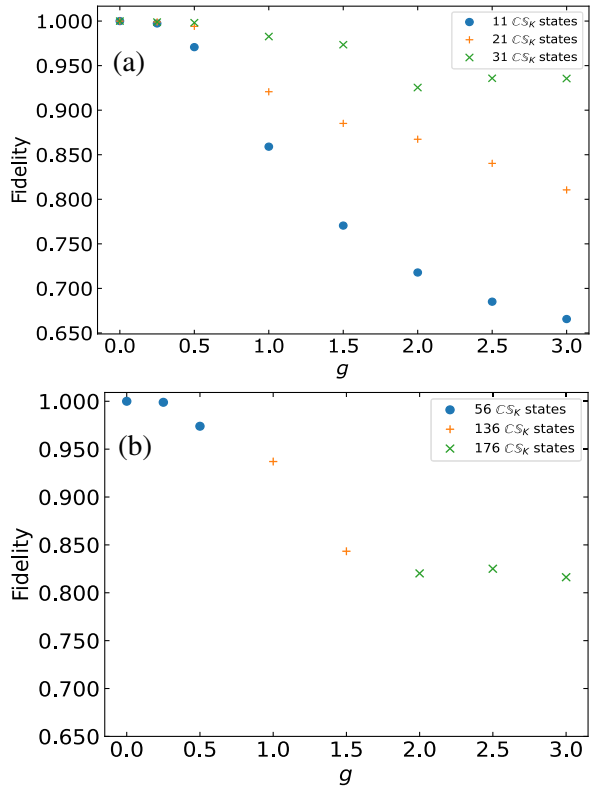

FIG. 2. Results for the transverse field Ising model with local dissipators described in the main text. The corresponding fidelity value between the state obtained and the theoretical state, for $\mathbb{CS}_K$ *Ansatz* of different *Ansatz* sizes K, are compared. (a) Results for 5 qubits. (b) Results for 8 qubits. For larger g, we note that the exact NESS becomes much less sparse. To continue to obtain good fidelities in this regime, we require larger number of states in our *Ansatz*.

Here $|\psi_\alpha^{(k)}\rangle$ are the eigenvectors of the unitary U which characterize the system's strong symmetry. The corresponding eigenvalues are $u_\alpha, \alpha \in [1, n_U]$, where $1 \leq n_U \leq D$ is the number of distinct eigenvalues of U, and $k \in [1, d_\alpha]$, where d_α is the dimension of the subspace corresponding to the eigenvalue u_α. This decomposition can be extended to the operator space $\mathcal{B}(\mathcal{H})$, through

$$\mathcal{B}(\mathcal{H}) = \bigoplus_{\alpha=1}^{n_U} \bigoplus_{\beta=1}^{n_U} \mathcal{B}_{\alpha\beta}, \tag{6}$$

where $\mathcal{B}_{\alpha\beta} = \mathrm{Span}\{|\psi_\alpha^{(n)}\rangle\langle\psi_\beta^{(m)}|\}$, $n \in [1, d_\alpha]$, $m \in [1, d_\beta]$. Each orthogonal subspace can contribute to the NESS solution, since each subspace $\mathcal{B}_{\alpha\beta}$ can have a solution $\rho_{\alpha\beta}$ such that $L[\rho_{\alpha\beta}] = 0$. Hence, our algorithm finds a solution which is a linear combination of the solutions from all the $\mathcal{B}_{\alpha\beta}$ subspaces. We note that physical density matrices (with unit trace) can only exist in the diagonal sub spaces $\mathcal{B}_{\alpha\alpha}$ due to the orthogonality between the eigenvectors from different $\mathcal{H}_\alpha$. However, precisely because the unphysical density matrices from $\mathcal{B}_{\alpha\beta}, \alpha \neq \beta$, have trace 0, they can contribute to physical solutions found by forming linear combinations with a physical density matrix, which changes physical properties of the solution. There are at least n_U physical, distinct NESSs, which we label as ρ_α^*, where $\rho_\alpha^* \in B_{\alpha\alpha}$. If another strong symmetry is present, these n_U different ρ_α^* can be further decomposed into NESSs from the new symmetry sectors.

Generalization of our method for multiple NESSs.—We can systematically obtain all the physical steady states that exist in all the symmetry subspaces for quantum systems with multiple steady states, if we have knowledge of the full Lindbladian. The simplest way would be to directly construct an *Ansatz* that lies in the desired symmetry subspace. If we have the capacity on the quantum computer to generate such states, which has been demonstrated for Dicke states [77] and states that conserve total magnetization in the XXZ Heisenberg chain [78], we can simply generate such a set of states and use that to construct our hybrid *Ansatz* for our algorithm. This method has the added advantage of reducing the size of the *Ansatz*, due to the reduction of the possible solution space. For example, we used the quantum circuit proposed in Ref. [78] for the 8-qubit XXZ Heisenberg chain with dephasing noise and obtained a fidelity of nearly 1 to the theoretical NESS in the $m = 4$ symmetry subspace with only 28 states in our *Ansatz*. Here, m is the eigenvalue of the total magnetization operator M. However, this method is limited due to difficulty in devising circuits that conserve a general symmetry. Thus, we also propose two general methods to find multiple NESSs.

The first method utilizes the SDP structure of the optimization. For each operator N_k that corresponds to the kth strong symmetry in our system, a NESS is found that is in the symmetry subspace corresponding to a particular eigenvalue n_k of N_k, by including the linear constraint $\mathrm{Tr}(\beta\tilde{N}_k) = n_k$ in the SDP, where $(\tilde{N}_k)_{ij} = \langle\chi_i|N_k|\chi_j\rangle$. These additional linear constraints are additional, efficiently implementable, hyperplanes in the parameter space that the optimizer needs to fulfill.

As an example, we consider a XXZ Heisenberg chain on a system with n qubits, $H_{XXZ} = \sum_{j=1}^{n-1} \sigma_X^j\sigma_X^{j+1} + \sigma_Y^j\sigma_Y^{j+1} + \Delta\sigma_Z^j\sigma_Z^{j+1}$, and dephasing noise, defined by the n jump operators $L_i = \sigma_Z^i$. The total magnetization $M = \sum_{i=1}^n \sigma_Z^i$ commutes with the Hamiltonian and all jump operators L_i, generating a strong symmetry given by $S_z = e^{i\phi M}$. This gives rise to $n + 1$ magnetization blocks, each associated with an eigenvalue of M and has its own unique NESS.

Considering the additional constraint $\mathrm{Tr}(\beta\tilde{M}) = m$, where $\tilde{M}_{ij} = \langle\chi_i|M|\chi_j\rangle$, our first method is able to obtain a solution which is in the m magnetization symmetry sector of M that agrees with the exact results. We emphasize that the usage of the quantum computer scales linearly with the number of constraints, as we do not need to measure the D, E, F, R matrices several times.

The second method does not require us to add additional constraints into the SDP, which allows our classical postprocessing to be more numerically stable. It utilizes the structure of a Vandermonde matrix to systematically remove the contributions from unwanted subspaces by applying the symmetry operator to the state and is discussed in detail in the Supplemental Material [45].

Conclusion.—We present a new algorithm for finding NESS solutions of open systems. Our approach restates the NESS problem as a feasibility SDP, which is a well-known and well-characterized optimization problem. We believe that this is the first work to apply this approach to solving master equations. As a consequence of our approach, we are able to utilize NISQ devices to aid a classical computer in its calculation, by offloading the difficult task of calculating expectation values of arbitrary Pauli strings to the quantum computer. Utilizing this quantum-assisted approach to NISQ devices, our algorithm retains all of the advantages that such algorithms have over competitors that rely on variationally optimizing a quantum circuit.

Our algorithm provides three main advantages over its NISQ competitors. Firstly, since it frames the NESS problem as a feasibility SDP, it allows us to bypass many of the problems associated with traditional variational quantum algorithms on NISQ devices, such as the barren plateau problem and training over the nonconvex landscape in the state space. Secondly, it provides a natural way to enforce the positivity constraint of density matrices during the optimization, along with any other constraints we would want to implement. One example where being able to enforce other constraints is useful is when multiple steady states exist. Lastly, our method also gives us a systematic way to increase the expressibility of our *Ansatz* without sacrificing trainability.

Our work opens up many avenues for research. NISQ devices are already utilized to study the ground states of chemical substances [79]. Most believe that studying open system many-body Hamiltonians, like the fermionic Hubbard model in the presence of generic dissipations, is classically intractable [80]. It is hoped NISQ devices and NISQ algorithms can make the simulation of such problems possible [81]. Our method extends these studies to open quantum systems and widens the range of applications. Furthermore, we believe our method can be used as a tool to assist environmental engineering [82] of open quantum systems. Studying how noise and *Ansatz* choice affects quantum-assisted methods such as ours are interesting problems to consider in the future. We believe it is possible to extend our algorithm to allow constraints over continuous variables, which changes the optimization program into a semi-infinite feasibility problem [83]. We expect all of these to have a substantial impact on the NESS problem in the near and far term.

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