

Variational Matrix Product Operators for the Steady State of Dissipative Quantum Systems

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We present a new variational method based on the matrix product operator (MPO) ansatz, for finding the steady state of dissipative quantum chains governed by master equations of the Lindblad form. Instead of requiring an accurate representation of the system evolution until the stationary state is attained, the algorithm directly targets the final state, thus, allowing for a faster convergence when the steady state is a MPO with small bond dimension. Our numerical simulations for several dissipative spin models over a wide range of parameters illustrate the performance of the method and show that, indeed, the stationary state is often well described by a MPO of very moderate dimensions.

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Introduction.—The physics of quantum systems out of equilibrium poses unsolved fundamental questions relating to nature at extreme conditions and to the dynamics after long time evolution. Progress in this field is, however, hard to achieve, due to the lack of analytical tools to solve many such problems and the limitations of existing numerical methods.

In recent times, growing attention has been directed to the out-of-equilibrium physics of open quantum systems, i.e., systems in interaction with an environment. This interest has been intensified by the potential applications to the fields of condensed matter physics, statistical physics, and quantum information processing [1–4]. In particular, it has been shown that dissipation can be used to engineer interesting quantum many-body states and to perform universal quantum computation [1,5], ideas which can be explored in the context of current experimental setups based on atomic systems [6]. A particularly interesting topic is that of dissipative quantum phase transitions (DQPTs), namely, transitions in the nonequilibrium steady state of an open system, which may arise from the competing effects of the Hamiltonian and the dissipative terms of the dynamics. An archetypical example is that of the model [7,8], but DQPTs have also been studied in fermionic [9–11], bosonic [12], and quantum spin systems [13–15].

Finding the stationary state of a generic master equation is not easy, even for 1D systems. Analytical treatment is limited to very specific problems, such as quadratic fermionic models [16] or systems under special conditions or approximations [17,18], and most often numerical techniques are necessary.

As in the case of pure states, an exact numerical treatment is possible only for small systems due to the exponentially growing computational cost, which may be even more severe in the case of mixed states. For pure states, parametrizing the state as a tensor network [19–21]

has proven an efficient alternative that can successfully capture the physical properties of quantum many-body states in countless situations of interest. The best example is the tremendous success of the density matrix renormalization group (DMRG) [22,23] based on the matrix product state (MPS) ansatz, which provides a quasixact solution for one-dimensional problems. The MPS can accurately describe ground states of gapped local Hamiltonians [24,25], and methods have been defined to use them also in real time evolution [26–29]. In combination with quantum trajectories, the latter have also been applied to dissipative dynamics [30]. The natural extension to operators, namely, matrix product operators (MPOs), can be used as an ansatz for mixed states [31,32], which is known to accurately describe thermal equilibrium states for local Hamiltonians [33,34]. Such an extension, in combination with the time evolution algorithms, has allowed the numerical exploration of steady states of spin chains and other one-dimensional systems under local dissipation (see, e.g., Refs. [3,35–40]).

This method is formally similar to the search for a ground state using imaginary time evolution [26], in that a given initial state is evolved until reaching a fixed point of the dynamics. However, different from the imaginary time evolution method, where the sequence of states visited by the algorithm is not of physical significance, in the simulation of a master equation, the real evolution needs to be followed so that errors in the intermediate state can severely affect the convergence of the procedure.

A better alternative could be given by a variational method, which searches for the null vector of the Lindblad superoperator within the MPO family, in the spirit of the DMRG variational search. Such a method would be potentially more efficient than simulating the full evolution, especially when the latter traverses intermediate states with a large bond dimension, but the true steady state is

described by a small one, as is often the case [3,36,41]. In this Letter, we present such variational method for the steady state of a master equation in Lindblad form. We illustrate the performance of the algorithm with results for several one-dimensional models. Notice that a variational method, similar in spirit but restricted to density matrices containing only few-body correlations, has been recently proposed in Ref. [42].

Basic concepts.—A MPS for a quantum system of Nd -dimensional components is a state vector of the form $|\Psi\rangle = \sum_{\{s_i\}} \text{tr}(A_1^{s_1} \dots A_N^{s_N}) |s_1 \dots s_N\rangle$ [43], where each A_i is a $d \times D \times D$ tensor, D is a parameter of the representation called bond dimension, and the sum runs over all elements of each individual basis $s_i = 1, \dots, d$. By successively increasing the bond dimension D , the MPS family defines a hierarchy of states covering vector space spanned by the tensor product of the individual bases, $\{|s_i\rangle\}$. The same ansatz can be used to represent operators whose coefficients in a tensor product basis have the structure of a matrix product, $\hat{O} = \sum_{\{s_i, r_i\}} \text{tr}(A_1^{s_1 r_1} \dots A_N^{s_N r_N}) |s_1 \dots s_N\rangle \langle r_1 \dots r_N|$. These are called MPOs [31,32,44]. The operators can be vectorized using Choi's isomorphism $|s_i\rangle \langle r_i| \rightarrow |s_i r_i\rangle$, which maps any operator \hat{O} to a vector $|\Phi(\hat{O})\rangle$, so that it is possible to work in the vector space of operators with the usual MPS techniques.

In order to describe physical mixed states, MPOs or, in this case, matrix product density operators (MPDOs), have to satisfy additional conditions; namely, they have to be normalized ($\text{tr}\rho = 1$), Hermitian, and positive semidefinite. While the first two conditions are easy to impose on the local tensors of the ansatz, the positivity involves the full spectrum of the operator and is, thus, a nonlocal property. The ansatz can be modified to represent positive operators using a local purification of the state with MPS structure. In this case, each tensor has a structure $A_n^{ij} = \sum_k X_n^{ik} \otimes \bar{X}_n^{jk}$, where the index k sums over the ancillary degree of freedom, and the bar indicates complex conjugation. Although it guarantees positivity, working with the purification ansatz is, in general, computationally more costly [45], and, moreover, the bond dimension required to write the purification ansatz may be much larger than that of the MPO [46] so that in practice it is not always the most convenient choice.

A variational search for the steady state.—We consider a chain of length N , with a quantum system of physical dimension d on each site and dynamics governed by a master equation of Lindblad form $\frac{d\rho}{dt} = \mathcal{L}[\rho]$, where the rhs is the Lindbladian superoperator,

$$\mathcal{L}[\rho] = -i[H, \rho] + \sum_{\alpha} \frac{1}{2} (2L_{\alpha}\rho L_{\alpha}^{\dagger} - \{L_{\alpha}^{\dagger}L_{\alpha}, \rho\}). \quad (1)$$

The unitary part of the evolution is determined by the system Hamiltonian, H . The effect of the environment is described by a set of Lindblad operators, L_{α} .

The Lindbladian acts linearly on the vectorized ρ as

$$\hat{\mathcal{L}} = -i(H \otimes \mathbb{1} + \mathbb{1} \otimes H) + \sum_{\alpha} \frac{1}{2} (2L_{\alpha} \otimes \bar{L}_{\alpha} - L_{\alpha}^{\dagger} L_{\alpha} \otimes \mathbb{1} - \mathbb{1} \otimes L_{\alpha}^T \bar{L}_{\alpha}). \quad (2)$$

The steady state is a fixed point of the evolution ($d\rho_s/dt = 0$) and corresponds to a vector $|\Phi(\rho_s)\rangle$ satisfying $\hat{\mathcal{L}}|\Phi(\rho_s)\rangle = 0$, i.e., a zero eigenvector of $\hat{\mathcal{L}}$. If the Hamiltonian and the individual Lindblad operators have local character, the Lindbladian can be written as a MPO (strictly speaking, it is enough that H and each L_{α} can themselves be written as MPOs, which include short-range interactions and dissipation but can also be applied to approximate power-law decaying terms [44]), and we can search for the best MPS approximation to its zero eigenvector, which will give us a vectorized MPO approximation for the steady state. Since the operator (2) is not Hermitian, in order to use the standard variational search with the MPS, we consider instead the Hermitian product $\hat{\mathcal{L}}^{\dagger} \hat{\mathcal{L}}$. The steady state is also a zero eigenvector of this operator, and, since $\hat{\mathcal{L}}^{\dagger} \hat{\mathcal{L}} \geq 0$, it corresponds to the lowest eigenvalue. If $\hat{\mathcal{L}}$ can be written as a MPO, the product can also, and it is then possible to use standard MPS algorithms to approximate its ground state [20,23]. Notice the particular case of Hermitian L_{α} is especially easy, since the (properly normalized) identity is a steady state, which can be exactly written as a MPS with bond dimension $D = 1$.

The fact that we are targeting density matrices requires particular attention because not every MPS vector can represent a valid physical state. The normalization condition $\text{tr}\rho = 1$ translates to $\langle \Phi(\mathbb{1}) | \Phi(\rho) \rangle = 1$, where $|\Phi(\mathbb{1})\rangle$ is the (unnormalized) vector that corresponds to the trace map, namely, the maximally entangled $|\Phi(\mathbb{1})\rangle = \sum_{\{s_i\}} |s_1 \dots s_N\rangle \otimes |s_1 \dots s_N\rangle$. A solution which is not orthogonal to this vector can always be normalized to ensure the trace condition. In general, it is more complicated to decide whether a MPS corresponds to a positive operator, since we do not have access to the full spectrum. The purification ansatz can guarantee that the search runs over only positive operators but at the expense of more costly local optimizations [45]. Hence, we use simply the vectorized MPO form and rely on the mathematical properties of the problem to provide a physical solution. Since the evolution generated by \mathcal{L} is a CP map, it must have a positive fixed point so that if this is nondegenerate, the algorithm should naturally converge towards a MPO approximation of a positive (and, hence, Hermitian) operator [strictly speaking, this may fail if the algorithm gets stuck in local minima or if there are degeneracies, as is known to happen also for DMRGs (see, e.g., Ref. [47])], and it is then expected to be almost positive, with any nonpositiveness being compatible with the truncation error.

In practice, we find that a suitable warm-up phase (see the Supplemental Material [48]) allows us to avoid solutions

with vanishing trace and improves the convergence of the algorithm. (Notice that it is also possible to use a Lagrange multiplier term of the form $|\Phi(\mathbb{1})\rangle\langle\Phi(\mathbb{1})|$ to favor solutions with nonvanishing trace. This can be subtracted from $\hat{\mathcal{L}}^\dagger\hat{\mathcal{L}}$, thus, increasing in one unit the bond dimension of the MPO. In practice, we found that the warm-up phase was enough to obtain physical solutions without increasing the computational cost.) Although positivity cannot be checked explicitly (it is, in fact, a hard problem [50]), there is a number of necessary criteria that any physical state needs to satisfy, such as physically sensible values of all single-body observables. Our algorithm performs a set of such tests and only accepts solutions that pass them all, otherwise, restarting the search with a different initial guess. The role of our consistency checks is to discard the least suitable guesses during the warm-up phase in order to prepare a suitable initial state for the variational search. During the later phases of the algorithm, the tests are used as assertions, while we rely on the convergence criteria (including that of the effective energy) to stop the calculation. After finding an acceptable solution for a given bond dimension D , we compute the desired expectation values from the Hermitian part of the MPO $(\rho + \rho^\dagger)/2$, as often done in other algorithms to reduce numerical errors (the norm of the non-Hermitian part can also be used as additional consistency check). The found solution is normalized and used as an initial guess for a larger bond dimension, and finally convergence in D is decided when the targeted observables are converged to the desired precision.

The algorithm as described here is, thus, formally equivalent to the variational ground-state search for a MPO Hamiltonian over the MPS family and presents the same scaling, only with d^2 playing the role of the physical dimension, and with an effective Hamiltonian which has the squared bond dimension of the MPO for $\hat{\mathcal{L}}$. The gap of $\hat{\mathcal{L}}^\dagger\hat{\mathcal{L}}$ will be the determinant for the convergence of the algorithm. It is interesting to notice that this is not related to the eigenvalues of $\hat{\mathcal{L}}$ but to its (squared) singular values (see Ref. [48]). All in all we, find that for typical cases, the small bond dimension required to approximate the steady state as a MPO compensates for the additional computational effort associated to $\hat{\mathcal{L}}^\dagger\hat{\mathcal{L}}$, provided the Lindbladian is not degenerate.

Another variational approach has been recently proposed [42], which chooses to minimize the trace norm of $\mathcal{L}[\rho]$. Since this quantity is not efficiently computable, the method in Ref. [42] proceeds by minimizing an upper bound to this norm for restricted sets of density matrices. Our eigenvalue minimization is, instead, equivalent to finding the vector that minimizes the Euclidean norm $\|\hat{\mathcal{L}}|\Phi(\rho)\rangle\|$ with the constraint $\|\Phi(\rho)\| = 1$. Both minimizations have an exact solution in the physical steady state, although they are not equivalent when not exactly on the stationary state. Using the Euclidean norm of the vectorized expression is preferable in our case, because

the trace norm requires the full diagonalization of the operators, impossible for the system sizes we are interested in, while the norm of the vectorized operators is efficiently calculable for the MPS ansatz.

Numerical results.—results. To illustrate the performance of the algorithm, we apply it to several spin chains, where the unitary and dissipative dynamics show competing effects regarding the coherence of the steady state.

Low-dimensional Dicke model.—results. A typical example of DQPT is exhibited by the Dicke model [7,8], in which the collective interaction with a single radiation mode induces coherent behavior on a system of N two-level atoms. The regime of parameters required to observe the DQPT is challenging, and the experimental observation of the phase transition has only been achieved recently [51–53]. It is, thus, interesting to understand the behavior of similar models which may then be easier to realize experimentally. We consider a chain of N two-level systems, where each pair of systems couples coherently to a common radiation mode. This can be represented by a spin-1/2 chain governed by a single-particle Hamiltonian $H = \sum_{i=1}^N g\sigma_i^x$ and Lindblad operators $L_i = \gamma(\sigma_i^- + \sigma_{i+1}^-)$, for $i = 1, \dots, N-1$, instead of the single collective Lindblad operator of the Dicke model so that this model can be considered a low-dimensional version of the latter. We study the nature of the steady state found by the algorithm at varying values of g/γ and increasing system sizes N up to 100, which allows us to perform a finite size extrapolation and study single-site observables and correlations in the thermodynamic limit. In the Dicke model, the superradiant phase transition (at $g/\gamma^2 = N$) [8] is visible in these observables. In the low-dimensional version, we do not find evidence of such transition, although (short-range) correlations appear, as shown in Fig. 1 for $S_y^2 = (\sum_i \sigma_i^y / N)^2$. It is remarkable that for all values $g/\gamma \geq 0.35$ and system sizes $N \leq 100$, the

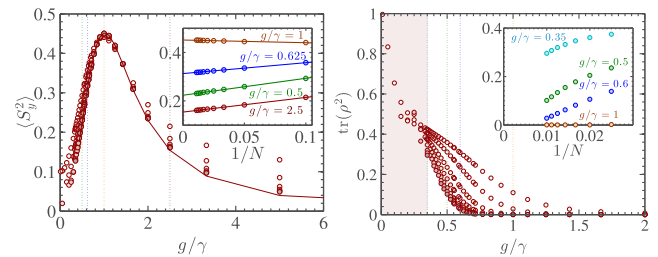


FIG. 1 (color online). Left: Correlation $\langle S_y^2 \rangle$ for the low-dimensional Dicke model, as a function of g/γ for system sizes $N = 10-100$ (in increasingly darker shades). The solid line is the result of finite size extrapolation, linear in $1/N$, as explicitly shown in the inset for several values of g/γ . Right: Purity of the converged steady state for the same system sizes. For large dissipation (shaded region), we show only results for the smallest systems, for which the simple variational search converges reliably. The inset shows the explicit dependence of the purity on the system size for several coupling values.

steady state is converged with very small bond dimension $D < 30$, most of them even with $D \leq 20$. At $g = 0$, there are, however, two dark states, namely, $|0\rangle^{\otimes N}$ and $(1/\sqrt{N})\sum_{k=1}^N(-1)^k|0^{(k-1)}\dots 1\dots 0^{(N-k)}\rangle$. Hence, the null subspace of $\hat{\mathcal{L}}$ is fourfold degenerate. This hinders the convergence of the algorithm at very small g/γ , as the steady state is no longer the unique and positive zero eigenvector, and the warm-up strategy is not enough to guarantee a physical solution, except for the smallest system sizes ($N \leq 20$). For those converged cases, we can detect the peculiarity of this parameter region by analyzing the purity of the solution shown in Fig. 1. Indeed, we can find positive solutions with increasing purity, which can be up to 1 for $g = 0$ (notice that for $g = 0$, any mixture of both dark states will be a steady state, with purity in $[0.5, 1]$). In principle, one could complement the method with additional techniques to try and select the physical steady states (e.g., finding and then processing several orthogonal eigenstates, not necessarily physical) even for larger chains. Here we have, nevertheless, focused on the convergence in the most commonly occurring situation of a unique steady state, where the method can provide the largest gain by directly targeting a MPO with small bond dimension.

Dissipative Ising chain.—A complementary kind of model is one where the Hamiltonian dynamics induces correlations, for instance, an Ising chain, and the dissipation is purely local. We consider a nearest-neighbor Ising interaction $H = (V/4)\sum_{i<N}\sigma_i^z\sigma_{i+1}^z + \sum_i\{(\Omega/2)\sigma_i^x - [(V-\Delta)/2]\sigma_i^z\} + (V/4)(\sigma_N^z + \sigma_N^x)$ and local dissipation given by $L_i = \sqrt{\gamma}\sigma_i^+$, $i = 1, \dots, N$. Such a model has attracted considerable attention in recent years, as it can be effectively realized in atomic lattice systems using Rydberg states [15,54,55]. In order to compare to existing results in the literature [54], we fix $\gamma = 1$, $V = 5$, and $\Omega = 1.5$. We compute the steady state for systems up to $N = 50$ and study the squared of the staggered magnetization $M_z = \sum_i(-1)^i\sigma_i^z/N$ equivalent to the antiferromagnetic order parameter defined in Ref. [54] and the purity of the steady state as a function of Δ (Fig. 2). We find that our convergence criteria are met with small bond dimension $D \leq 20$. Our results show the order parameter vanishing as $N \rightarrow \infty$, consistent with short-range correlations, which, indeed, are observed to decay exponentially. We observe that the purity of the steady state grows for large absolute values of Δ . This can be easily understood by going to the interaction picture with respect to the single body σ_i^z terms in the Hamiltonian. This does not change the form of the dissipative terms, but for very large $|V - \Delta|$, the σ_i^x terms can be neglected in the rotating wave approximation. In this situation, the single dark state of the dissipation, the fully polarized state $|0\rangle^{\otimes N}$, is also an eigenstate of the Hamiltonian and is, thus, a steady state.

The method can also be applied to other models, for instance, with coherence induced by both the Hamiltonian and the environment [48].

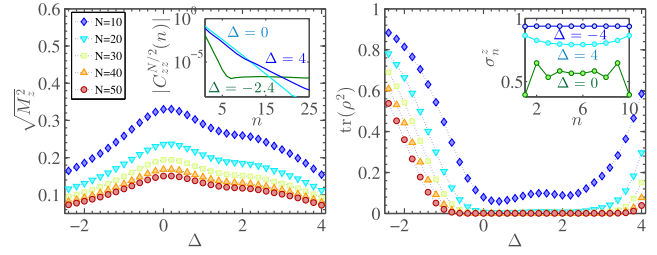


FIG. 2 (color online). Left: Antiferromagnetic order parameter $\sqrt{\langle M_z^2 \rangle}$ in the steady state of the Ising model with local dissipation, for several system sizes, and fixed $\gamma = 1$, $V = 5$, $\Omega = 1.5$, as a function of Δ . The inset shows the exponential decay of correlations $C_{zz}^{N/2}(n) = \langle \sigma_{N/2}^z \sigma_{N/2+n}^z \rangle - \langle \sigma_{N/2}^z \rangle \langle \sigma_{N/2+n}^z \rangle$, for $N = 50$ in the various regions of Δ . Right: Purity of the converged steady state for the same system sizes. The inset shows the local polarization σ_n^z for the $N = 10$ case. At $\Delta = 0$, the antiferromagnetic ordering can be appreciated, while for larger values of $|\Delta|$, the steady state approaches total polarization.

Conclusion.—We have presented and analyzed a variational algorithm that searches for a MPO approximation to the steady state of an open quantum system. The algorithm is applicable to any model in which the Hamiltonian and the Lindblad operators can be expressed as MPOs. Instead of simulating the real time evolution of the system, as done by other existing tensor network approaches, this method directly targets the stationary state, without the need to precisely describe intermediate states which may need a larger bond dimension than the actual solution. Thus, our technique can allow for a more efficient exploration of the steady-state phase diagram. Our numerical results have shown that for a varied set of models, with correlations created by the unitary evolution, the dissipation or both [48], the steady state is, indeed, well approximated by a MPO of very small bond dimension $D \leq 30$ for sizes up to $N = 100$. This can be directly compared to the bond dimensions required to describe the intermediate states in time evolution methods. For instance, in Ref. [56] $D \approx 200$ was required for a dissipative Ising chain of length $N = 40$. In Ref. [3], the evolution required D of several hundreds [57] for an XXZ chain of length $N = 96$ when the steady state has $D = 1$.

Our approach is based on the ground-state optimization over the MPS for a MPO Hamiltonian and relies on the guaranteed existence of a valid, positive steady state. This basic technique is complemented with a warm-up phase or a suitable initial guess found to be crucial in practice for convergence to a physical result with small bond dimension.

When the steady state is degenerate, the simplest method described in this Letter might have problems to find a valid guess for the steady state. In particular, in the situation of several dark states, the null subspace of the Lindbladian contains infinitely many vectors which do not correspond to positive operators and, hence, do not constitute valid

physical states (notice that this situation could also be adverse for time evolving numerical methods). In principle, it would be possible to complement the current algorithm with additional techniques, such as symmetries, in order to reduce the degeneracy, or to construct a candidate steady state from appropriate combinations of several linearly independent null vectors, even if nonpositive.

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