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.

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 (DQPT), namely transitions in the non-equilibrium 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 Dicke model [7, 8], but DQPT have also been studied in fermionic [9, 10], bosonic [11] and quantum spin systems [12–14].

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 [15], or systems under special conditions or approximations [16, 17], 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 (TN) [18–20] 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) [21, 22], based on the matrix product state (MPS) ansatz, which provides a quasi-exact solution for one dimensional problems. MPS can accurately describe ground states of gapped local Hamiltonians [23, 24], and methods have been defined to use them also in real time evolution [25–28]. In combination with quantum trajectories, the latter have also been applied to dissipative dynamics [29].

The natural extension to operators, namely matrix product operators (MPO), can be used as an ansatz for mixed states [30, 31], which is known to accurately describe thermal equilibrium states for local Hamiltonians [32, 33]. 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. [3, 34–39]). This method is formally similar to the search for a ground state using imaginary time evolution [25], in that a given initial state is evolved until reaching a fixed point of the dynamics. However, different to the imaginary time evolution method, 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, specially when the latter traverses intermediate states with a large bond dimension, but the true steady state is described by a small one. In this paper 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 [40].

BASIC CONCEPTS

A matrix product state (MPS) for a quantum system of $N$ $d$-dimensional components, is a state vector of the form $|\Psi\rangle = \sum_{\{s_i\}} \text{tr} \left(A_{s_1}^N \cdots A_{s_N}^N |s_1 \cdots s_N\rangle\right)$ [41], 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 el-
elements of each individual basis $s_i = 1, \ldots, d$. 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, $O = \sum_{(s_i, r_i)} \text{tr}\left(A^{s_i r_i}_{1} \cdots A^{s_N r_N}_{N}\right) \{|s_1 \ldots s_N\rangle\langle r_1 \ldots r_N|\}$. These are called matrix product operators (MPO) [30, 31, 42].

The operators can be vectorized using Choi’s isomorphism, $|s_i\rangle\langle r_i| \rightarrow |s_i r_i\rangle\langle r_i s_i|$, which maps any operator $\hat{O}$ to a vector $|\Phi(O)\rangle$, 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, MPO, or in this case matrix product density operators (MPDO), have to satisfy additional conditions, namely they have to be normalized ($\langle \rho \rangle = 1$), 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 non-local 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 $A^{\alpha}_{n} = \sum_k X^n_k \otimes X^n_k$, 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 [43] and moreover the bond dimension required to write the purification ansatz may be much larger than that of the MPO [44], 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,

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

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, $L_\alpha$.

The Lindblad acts linearly on the vectorized $\rho$, as

$$\frac{d\rho}{dt} = -i (H \otimes \mathbb{1} + \mathbb{1} \otimes H) \rho + \sum_\alpha \frac{1}{2} \left( 2L_\alpha \otimes L_\alpha^\dagger - L_\alpha^\dagger L_\alpha \otimes \mathbb{1} - \mathbb{1} \otimes L_\alpha^\dagger L_\alpha \right).$$

The steady state is a fixed point of the evolution, $\frac{d\rho}{dt} = 0$, and corresponds to a vector $|\Phi(\rho_s)\rangle$ satisfying $\mathcal{L}[\Phi(\rho_s)] = 0$, i.e. a zero eigenvector of $\mathcal{L}$. If the Hamiltonian and the individual Lindblad operators have local character, the Lindbladian can be written as a MPO, 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 MPS we consider instead the Hamiltonian product $\mathcal{L} L \mathcal{L}$. The steady state is also a zero eigenvector of this operator, and, since $\mathcal{L} L \mathcal{L} \geq 0$, it corresponds to the lowest eigenvalue. If $\mathcal{L}$ can be written as a MPO, also the product can, and it is then possible to use standard MPS algorithms to approximate its ground state [19, 22]. Notice the particular case of Hermitian $L_\alpha$ 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 $|\Phi(\mathbb{1})\rangle = \sum |s_1 \ldots s_N\rangle \otimes |s_1 \ldots s_N\rangle$. 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 [43]. 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 non-degenerate, the algorithm should naturally converge towards a MPO approximation of a positive (and hence Hermitian) operator and is then expected to be almost positive, with any non-positive ness being compatible with the truncation error.2

In practice, we find that a suitable warmup phase (see Appendix ) allows us to avoid solutions with vanishing trace, and improves the convergence of the algorithm.3 Although positivity cannot be checked explicitly (it is in fact a hard problem [45]), 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. After finding an acceptable solution for a given bond dimension, $D$, we ensure hermiticity by retaining the hermitian part of the MPO, $(\rho + \rho^\dagger)/2$. The solution found is normalized and used as initial guess for a larger bond dimension, and finally con-

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1 Strictly speaking, it is enough that $H$ and each $L_\alpha$ can themselves be writ-

2 Strictly speaking, this may fail if the algorithm gets stuck in local minima, or if there are degeneracies. Notice that it is also possible to use a Lagrange multiplier term, of the form $|\Phi(\mathbb{1})\rangle (\Phi(\mathbb{1})\rangle$, to favor solutions with non-vanishing trace. This can be subtracted from $\mathcal{L} L \mathcal{L}$, 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.
verges reliably. The inset shows the explicit dependence of the purity 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.

Low dimensional Dicke model. 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 [46, 47]. 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, $H = \sum_{i=1}^{N} g\sigma_i^z$, and Lindblad operators $L_i = \gamma(\sigma_i^+ + \sigma_{i+1}^-)$, for $i = 1, \ldots, N-1$, 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 $g/\gamma$ 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 figure 1 for $S_\Delta^2 = \sum_{k=1}^{N} g\sigma_k^2/N$. It is remarkable that for all values $g/\gamma \geq 0.35$ and system sizes $N \leq 100$ the 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 $\frac{1}{\sqrt{N}} \sum_{k=1}^{N} (-1)^k |0_{(-k)} ... 1 \ (N-k) \ 0\rangle$.

Hence, the null subspace of $\hat{L}$ is four-fold degenerate. This hinders the convergence of the algorithm at very small $g/\gamma$, as the steady state is no longer the unique and positive zero eigenvector, and the warmup 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 figure 1. Indeed, we can find positive solutions with increasing purity, which can be up to 1 for $g = 0$. 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, $H = \frac{V}{4} \sum_{i} \sigma_i^z \sigma_{i+1}^z + \sum_i \left( \frac{1}{2} \sigma_i^+ \sigma_i^- + \frac{V}{2} \sigma_i^z \right) + \frac{V}{4} (\sigma_i^z + \sigma_N^z)$, and local

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4 Notice that for $g = 0$ any mixture of both dark states will be a steady state, with purity in $[0.5, 1]$. 

**FIG. 1.** Left: Correlation $\langle S_\Delta^2 \rangle$ for the low dimensional Dicke model, as a function of $g/\gamma$ for system sizes $N = 10 \ldots 100$ (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 $g/\gamma$. 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.
dissipation given by $L_i = \sqrt{\gamma} \sigma^z_i$, $i = 1, \ldots, N$. Such a model has attracted considerable attention in recent years, as it can be effectively realized in atomic lattice systems using Rydberg states [14, 48, 49]. In order to compare to existing results in the literature [48], we fix $\gamma = 1$, $V = 5$, $\Omega = 1.5$. We compute the steady state for systems up to $N = 50$ and study the squared of the staggered magnetization, $M_z = \sum_i (-1)^i \sigma^z_i / N$, equivalent to the antiferromagnetic order parameter defined in [48], and the purity of the steady state as a function of $\Delta$. Fig. 2, and the purity of the steady state as a function of $\Delta$ (Fig. 2). We find that our convergence criteria are met with small bond dimension $D < 20$. Our results show the order parameter vanishing as $N \to \infty$, 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 $\Delta$. This can be easily understood by going to the interaction picture with respect to the single body $\sigma^z_i$ terms in the Hamiltonian. This does not change the form of the dissipative terms, but for very large $|V - \Delta|$, the $\sigma^z_i$ 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.

**Ising chain with coherent dissipation.** Finally, we test the algorithm on a model where both the Hamiltonian and the dissipative dynamics can induce coherence. Namely, we study an Ising model, $H = \sum_i \sigma_i^z \sigma_{i+1}^z + g \sum_i \sigma_i^z$, with nearest neighbor Lindblad operators, $L_i = \mu \sigma_i^+ + \nu \sigma_{i+1}^-$, $i < N$ (plus $L_N = \mu \sigma_N^+$). For chains of up to $N = 50$ sites, we find convergence with remarkably small bond dimension, $D < 20$. Figure 3 illustrates the expectation value of $S_z^2 = (\sum_i \sigma_i^z)^2$ in the steady state for the particular case $\mu = 0.5$ and changing values of $g$ and $\nu$, after extrapolating the results to $N \to \infty$. It is easy to check that in the thermodynamic limit the identity is always a steady state for the symmetric case, $\mu = \nu$. This explains the vanishing $\langle S_z^2 \rangle$ observed in the plots when $\nu = 0.5$ for all values of $g$.

**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 MPO. 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 show that for a varied set of models, with correlations created by the unitary evolution, the dissipation or both, the steady state is indeed well approximated by a MPO of very small bond dimension.

Our approach is based on the ground state optimization over 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 paper might have problems to find a valid guess for the steady state. Specially 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. 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 non positive.

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5 Notice that this situation could also be adverse for time evolving numerical methods.
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APPENDIX: NUMERICAL DETAILS

In the variational search for the best MPS approximation to the ground state of a Hamiltonian, $H$, the optimization proceeds using an alternating least squares (ALS) strategy, in which the energy, $\langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle$, is successively minimized with respect to one of the tensors in the ansatz, while the remaining tensors are fixed [50]. In the case of the steady state optimization, the basic algorithm is identical, where the product $\hat{L}^{\dagger} \hat{L}$ plays the role of the Hamiltonian. We use a MPO description for the superoperator $\hat{L}$, which can be easily constructed as for the Hamiltonian case, so that also $\hat{L}^{\dagger} \hat{L}$ has a MPO representation with the squared bond dimension of the former (see figure 4). In particular, in the cases described in this work, the operator $\hat{L}$ contains only local and nearest-neighbor terms, but the construction can be extended to more general situations [42]. Running the ALS optimiza-
tion requires the corresponding effective operator on each tensor, i.e. the contraction of $\langle \Psi | \hat{L}^\dagger \hat{L} | \Psi \rangle$ except for this tensor, which can be computed efficiently using the same basic computational routines as the ground state algorithms.

The search for the ground state of $\hat{L}^\dagger \hat{L}$ can then produce a MPS approximation to the vector $|\Phi(\rho_s)\rangle$, normalized in Euclidean norm, which minimizes $\| \hat{L} | \Phi(\rho_s) \rangle \|$. But not every such approximation will represent a possible physical state, as those need to be positive operators, with trace one. Mathematically, there is a zero-eigenstate of $\hat{L}$ corresponding to a positive operator, so that the algorithm will in general be naturally looking for a physical solution (except in the case, illustrated in the main text, of several dark states). Nevertheless we identify some additional techniques that help ensuring the stability and fast convergence of the algorithm.

**Initial warmup phase.** In general it is convenient to start the variational search with a small bond dimension, $D$, and to use the result as initial guess for the search with increased $D$ until the required precision is attained. In the steady state case, nevertheless, if the initial bond dimension is very small, it might happen that the algorithm at this stage converges to some vector not corresponding to a physical state, which constitutes a bad initial guess for the next rounds. This may lead to very slow convergence, and to an artificial increase of the required bond dimension for the final solution. Hence, for the smallest bond dimension, instead of directly starting the algorithm on a random vector, we implement a first warmup phase that constructs a more suitable initial state. This is then fed to the usual DMRG-like sweep, until convergence. We also observe that the algorithm behaves better when the bond dimension is increased in small steps.

In particular, for the (close to) reflection symmetric models considered here, the first sweeps over the MPS tensors are not performed from left to right and back, as in the regular DMRG algorithms, but symmetrically from the outside in, or from the inside out. We find that this strategy works best when starting from the separable ansatz, $D = 1$, for which the algorithm is extremely fast, and can thus be made to converge to numerical precision, and be repeated if necessary at a low cost. If after the algorithm has converged for $D = 1$, if the solution is not compatible with a physical state, the procedure is repeated from a different initial state. Otherwise, the bond dimension is increased, and the obtained state is used as initial guess.\(^6\)

**Physical solutions.** Checking whether a given MPO corresponds to a physical operator is in general a very hard problem. Nevertheless, we can apply some compatibility checks to discard the most unphysical solutions. More concretely, for the spin-1/2 chains studied, we demand that each of the local magnetizations, $\sigma_n^x, \sigma_n^y, \sigma_n^z$, have expectation values within the physical range.\(^7\) We found this to be enough to identify the most unphysical intermediate solutions, and to obtain solutions with non-vanishing trace, so that the steady state could be properly normalized, but it is possible to define additional tests and perform more demanding physicality checks. Additionally, it might also be interesting to complement the minimization of $\hat{L}^\dagger \hat{L}$ with a Lagrange multiplier term to favor vectors that are not orthogonal to the identity.

**Deciding convergence.** For the ground state search, convergence of the global algorithm can be decided in terms of the relative variation of the energy from one value of the bond dimension to the next. In our case, the exact solution has zero eigenvalue. Instead of its relative variation, we check the absolute value, so we require that the found eigenvalue is below some threshold, and additionally, demand convergence of some physical observables. In particular, we require that the local polarizations converge, by constructing the $N$-component vectors, $(\sigma_1^\alpha, \ldots, \sigma_N^\alpha)$, for $\alpha = x, y, z$ and requiring that the relative variation (in Euclidean norm) when increasing the bond dimension is below $10^{-4}$. With these criteria, the steady state is converged for all the cases presented in this work. Additionally we check that other observables (such as the antiferromagnetic order parameter for the Ising model with local dissipation) and even the purity, which is far from being a local observable, are converged to a precision better than $10^{-2}$.

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\(^6\) When exploring the parameter space of a certain model, this technique can be used for some parameter values and then the converged results can be used as guesses for the model with slightly changed parameter.

\(^7\) At least within some tolerance, which can be relaxed for the smallest bond dimensions.