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Matrix Product Density Operators: Simulation of Finite-Temperature and Dissipative Systems

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We show how to simulate numerically the evolution of 1D quantum systems under dissipation as well as in thermal equilibrium. The method applies to both finite and inhomogeneous systems, and it is based on two ideas: (a) a representation for density operators which extends that of matrix product states to mixed states; (b) an algorithm to approximate the evolution (in real or imaginary time) of matrix product states which is variational.

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The physical understanding of quantum many-body systems is hindered by the fact that the number of parameters describing the physical states grows exponentially with the number of particles. Thus, even for a relatively small number of particles, most of the problems become intractable. During the last decade, however, several numerical methods have been put forward which allow us to describe certain many-body systems. One such method is the so-called density matrix renormalization group (DMRG), which is very well suited to describe 1D systems on a lattice with short-range interactions and at zero temperature [1–3]. In fact, DMRG has had a very strong impact in the field of condensed matter physics, allowing us to describe such systems with an unprecedented degree of accuracy and to extract their physical behavior.

Several years after its discovery, DMRG was extended to finite-temperature 1D systems [4]. The method applies to translationally invariant infinite systems, since in that case the evaluation of the partition function can be recast in terms of finding the maximum eigenvalue of a finite matrix, which in turn can be found using a variation of the original DMRG method to classical two-dimensional spin systems [5]. The main restriction of the method is that it does not work well for low temperatures and that it cannot be applied in situations in which the number of particles is finite and/or not homogeneous, as it is, e.g., the case of atoms in optical lattices [6]. Recently, time-dependent versions of the DMRG method have been put forward [7–10].

The success of the DMRG method and its extensions is based on the fact that the many-body states that appear in some 1D problems can be very well described in terms of the so-called matrix product states (MPS) [11–13], i.e.,

$$|\psi_{\mathrm{MPS}}\rangle = \sum_{s_1,\ldots,s_N=1}^{d} \mathrm{Tr}(A_1^{s_1}\ldots A_N^{s_N})|s_1,\ldots,s_N\rangle. \qquad (1)$$

Here, the A's are matrices whose dimension is bounded by some fixed number D and d is the dimension of the Hilbert space corresponding to the physical systems. In fact, DMRG can be viewed, both for finite and infinite dimensions, as an iterative method that for a fixed D determines the matrices whose state $|\psi_{\mathrm{MPS}}\rangle$ minimizes the energy in a variational sense [11,13]. On the other hand, the method introduced by Vidal in the context of simulating the dynamics of weakly entangled quantum systems [14] and later developed in [8–10] prescribes a particular way to update the matrices A as a function of time. This method can be extended [14] to determine the evolution of mixed states by considering them as vectors in the d^{2N}-dimensional space of linear operators and thus doubling the number of matrices A.

In this Letter, we introduce the notion of matrix product density operators (MPDO) which extend the MPS from pure to mixed states. We also present *the optimal* way in which the time evolution of pure and mixed states can be approximated within these two classes of states (MPS and MPDO). The corresponding evolution in imaginary time leads to a very versatile finite-T DMRG algorithm, not restricted to large temperatures or to homogeneous systems. We conclude by showing how dissipative systems governed by master equations can be efficiently simulated.

In [13,15,16], a picture was introduced to analyze MPS and DMRG from a quantum information perspective (see Fig. 2 in [13]). The MPS (1) can be depicted as being built up by a collection of virtual D-level systems paired in maximally entangled states. The MPS is obtained by applying linear maps which transform the D^2-dimensional Hilbert space of pairs of virtual systems into the local Hilbert spaces associated with the physical systems. Thus, the MPS is completely specified by these maps which in turn can be reexpressed in terms of the matrices A of Eq. (1). A central result of this Letter is that this picture can be extended to describe mixed quantum states. The idea is as follows: instead of applying a linear map to the Hilbert space associated with pairs of virtual systems, we apply a general completely positive map (CPM) to the corresponding operator space, which is the most general map allowed by quantum mechanics [17]. We hence define the class of MPDO as the class of states which can be obtained by this procedure. More specifically, a MPDO ρ of N d-level particles with $(D_1, D_2, \ldots, D_N)$-dimensional bonds is defined as

$$\rho = \sum_{s_1,s_1',\ldots,s_N,s_N'=1}^{d} \mathrm{Tr}(M_1^{s_1,s_1'} \ldots M_N^{s_N,s_N'})|s_1,\ldots,s_N\rangle \times \langle s_1',\ldots,s_N'|, \tag{2}$$

where $M_k^{s_k,s_k'}$ are $D_k^2 \times D_{k+1}^2$ matrices that can be decomposed as

$$M_k^{s,s'} = \sum_{a=1}^{d_k} A_k^{s,a} \otimes (A_k^{s',a})^*. \tag{3}$$

Here d_k is at most dD_kD_{k+1}, and the matrices $A_k^{s,k}$ are of size $D_k \times D_{k+1}$. Condition (3) is a semidefinite constraint and is sufficient to ensure that the associated map is completely positive. Relaxing this condition gives rise to operators which are not necessarily positive semidefinite (i.e., the picture introduced above also allows one to represent general operators). Note also that for sufficiently large D, Eq. (2) includes *any* density operator acting on the Hilbert space. For example, the maximally mixed state corresponds to the choice $M_k^{s,s'} = \delta_{s,s'}\mathbf{1}$, and a pure MPS is recovered when $M_k^{s,s'} = A_k^s \otimes (A_k^{s'})^*$.

It is possible to express any MPDO in terms of a (pure) MPS by defining the latter over a larger Hilbert space, i.e., by using the concept of purification [17]. With each physical system we associate an auxiliary system (or ancilla) with a Hilbert space of dimension d_k, and, after choosing an orthonormal basis $|s_k, a_k\rangle$ for these particle-ancilla pairs, we write the corresponding MPS state as

$$|\Psi\rangle = \sum_{s_1,\ldots,s_N} \sum_{a_1,\ldots,a_N} \mathrm{Tr}\left(\prod_{k=1}^{N} A_k^{s_k,a_k}\right)|s_1a_1,\ldots,s_Na_N\rangle. \tag{4}$$

The MPDO ρ is obtained after tracing over the ancillas, i.e., $\rho = \mathrm{Tr}_a(|\Psi\rangle\langle\Psi|)$. It is remarkable that for many interesting states the ancilla's dimensions can be chosen to be small ($d_k \simeq d$) and thus the purification (4) yields a very efficient representation of the MPDO. Note also that the ancilla matrices A_k in (4) can be easily recovered from the matrices M_k by means of an eigenvalue decomposition. On the other hand, given the matrices M_k, one can efficiently determine expectation values as follows:

$$\langle O_1 \ldots O_N\rangle_\rho = \mathrm{Tr}(E_{1,O_1} \ldots E_{N,O_N}), \tag{5}$$

where $E_{k,O} = \sum_{s,s'}\langle s'|O|s\rangle M_k^{s,s'}$.

In order to measure the error that we make when we approximate a density operator ρ_0 by some other one ρ, one can use different quantities. For instance [17], $E_F(\rho, \rho_0) = 1 - F(\rho, \rho_0)$, where F extends the notion of fidelity from pure to mixed states, it is defined as the maximal overlap between all possible purifications of ρ and ρ_0, and it is given by $F(\rho, \rho_0) = \mathrm{Tr}(\sqrt{\sqrt{\rho}\rho_0\sqrt{\rho}})$. Alternatively, we may simply take $E_{\mathrm{HS}}(\rho, \rho_0) = \mathrm{Tr}[(\rho - \rho_0)^2]$ which is related to the Hilbert-Schmidt scalar product in the space of operators.

If we want to determine a Hamiltonian time evolution of a mixed state in real or imaginary time, we may instead simulate the evolution of the purification. Starting out from the MPS purification $|\Psi(0)\rangle$ (4), we take a small time step and compute the next purification $|\Psi(\Delta t)\rangle$ exactly. Unless the evolution is local, the dimension of the matrices A will increase, and we will have to find a MPS that approximates the exact one, as in the method introduced in [8]. However, we do this here in an optimal way, i.e., we compute the MPS which, for given dimensions $\{D_k\}$, maximizes the overlap with the exact state. This "truncated" purification is taken as our next initial data, and we repeat the process. At any time, the purification can be used to reconstruct the density operator and to compute expectation values of observables.

Our method is based on an iteration which resembles the sweeps used in standard DMRG. Let us assume that we have $|\phi\rangle$, a MPS (1), and we want to find the closest one, $|\phi'\rangle$, in which the A's are replaced by $\tilde{A}$'s and the corresponding dimensions are $\tilde{D}_k \leq D_k$. Starting with a guess of the $\tilde{A}$'s (for example, the one of the previous step), on each step of the iteration we choose a site k and find the optimal $\tilde{A}_k$ such that the overlap between $|\phi\rangle$ and the MPS is maximal. The optimal choice is given by the solution of the system of equations

$$C_{\alpha,\beta}^{\alpha',\beta'}(\tilde{A}_k^s)_{\alpha',\beta'} = H_{\alpha,\beta}^s. \tag{6}$$

The tensors C and D are defined as

$$C_{\alpha,\beta}^{\alpha',\beta'} = \mathrm{Tr}(\Delta_{\alpha',\beta'} \otimes \Delta_{\alpha,\beta}E_{k+1} \ldots E_NE_1 \ldots E_{k-1}),$$
$$H_{\alpha,\beta}^s = \mathrm{Tr}(A_k^s \otimes \Delta_{\alpha',\beta'}G_{k+1} \ldots G_NG_1 \ldots G_{k-1}),$$

where $\Delta_{\alpha,\beta}$ is a matrix with a single nonzero element at row α and column β, and $E_k = \sum_s\tilde{A}_k^s \otimes (\tilde{A}_k^s)^*$, and $G_k = \sum_sA_k^s \otimes (\tilde{A}_k^s)^*$. Sweeping from $k = 1$ to N and back several times we reach always a fixed point with maximal overlap $|\langle\phi|\tilde{\phi}\rangle|$. The method becomes most efficient for open boundary conditions ($D_1 = D_{N+1} = 1$), as in that case orthonormality conditions can be imposed [13] such that $C_{\alpha,\beta}^{\alpha',\beta'} = \delta_{\alpha,\alpha'}\delta_{\beta,\beta'}$, and also $H_{\alpha\beta}^s$ can then be calculated very efficiently as in standard DMRG.

The recent time-evolution methods [8–10] developed in the context of DMRG seem to yield simulations that are quite close to the optimal method proposed here. A big advantage of our method, however, is that it can be formulated for periodic boundary conditions and that it can be generalized to the case of long-range interactions. The latter can be treated within our formalism as the algorithm also allows one to obtain a variational approximation of a sum of MPS by one MPS. Another advantage is that multiple Trotter steps can be implemented exactly in one truncation step.

Now we apply the previous ideas to approximate the density operator for a system at thermal equilibrium, i.e., $\rho \propto e^{-\beta H}$ with $\beta = 1/T$. For $\beta = 0$ (infinite temperature), the state ρ is a maximally mixed state $\mathbf{1}$. For any other temperature we use [18]

$$e^{-\beta H} = (e^{-\Delta t H})^M \mathbf{1} (e^{-\Delta t H})^M, \qquad \text{with } \Delta t = \tfrac{\beta}{2M}. \tag{7}$$

This means that we can obtain ρ by evolving according to the Hamiltonian in imaginary time, with time step Δt. This evolution can be performed by applying the optimal method presented above on the purification; in this case it is sufficient to fix the dimension of the ancilla to d, and hence the computational cost for open boundary conditions would scale as $(dD)^3$.

Using these techniques, we have computed the equilibrium states of a spin $s = 1/2$, XY model with transverse magnetic field

$$H_{xy} = \sum_{k=1}^{N} (\sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + h\sigma_k^z). \tag{8}$$

In Fig. 1(a) we plot the magnetization versus the magnetic field for four different temperatures, $N = 60$ spins. The accuracy of the matrix product representation seems to increase with temperature. Using smaller lattice sizes ($N = 8$ spins) and a fixed magnetic field ($h = 3.0$), we compared the exact diagonalization and the MPDO results for different dimensions, D. As Fig. 1(b) shows, no large D's are needed to describe the thermal states accurately. The main source of errors is due to the Trotter approximation, which can easily be cured by considering a higher order of Trotter decomposition.

Let us now move on to the description of the evolution of spin systems in the presence of decoherence, which is of interest in the context of experiments performed in atomic physics. For illustrative purpose, we consider a master equation of the form [19]

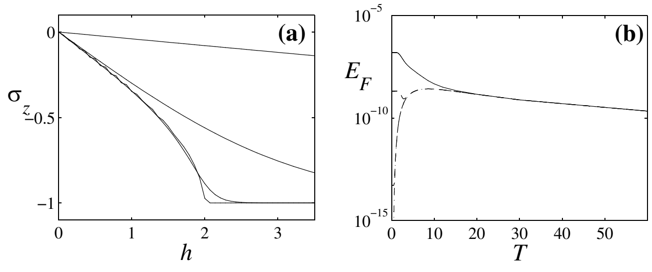

FIG. 1. (a) Magnetization vs transverse magnetic field of the thermal state of an XY model with 60 spins, for temperatures $T = 0.05$, 0.5, 5, and 50 (bottom to top). (b) Error in the density matrix of the thermal state of Eq. (8) computed using MPDO, vs temperature, for a chain with $N = 8$ spins, $D = 8$ (solid line) and $D = 14, 20, 24$ (dashed line).

$$\frac{d}{dt}\rho = i[H_z, \rho] + \gamma \sum_i (\sigma_i^x \rho \sigma_i^x - \rho) =: \mathcal{L}\rho, \tag{9}$$

where H_z is the Ising Hamiltonian mentioned before and γ characterizes the interaction with the environment; this master equation could, e.g., describe the evolution of atoms in an optical lattice, where the dissipative term is due to collisions with molecules.

Given an initial condition $\rho(0) = \rho_0$ written in MPDO form (2), we want to find the MPO which best approximates $\rho(t)$. The procedure that we propose resembles the one for Schrödinger equations, in that we integrate almost exactly the master equation for a short time Δt, and then find the optimal MPDO of smaller dimensions which is closest to $\rho(t + \Delta t)$. Let us denote by $\mathcal{E}(\mathcal{L}, t) = \exp(t\mathcal{L})$ the CPM so that $\rho(t) = \mathcal{E}(\mathcal{L}, t)\rho(0)$. We decompose this operator as follows:

$$\mathcal{E}(\mathcal{L}, \Delta t) \simeq [\mathcal{E}(\mathcal{L}_e, \Delta t/2)\mathcal{E}(\mathcal{L}_o, \Delta t)\mathcal{E}(\mathcal{L}_e, \Delta t/2)]^n, \tag{10}$$

where $\mathcal{L} = \mathcal{L}_o + \mathcal{L}_e$ is a splitting of the Liouvillian into commuting terms which act on odd, $(2k + 1, 2k)$, and even neighbors, $(2k, 2k + 1)$, respectively.

The action of the operators $\mathcal{E}(\mathcal{L}_e, \Delta t/2)$ or $\mathcal{E}(\mathcal{L}_o, \Delta t)$ on a state of the form (2) can be computed exactly, and one obtains an operator $\rho_o = \mathcal{E}(\mathcal{L}_o, \Delta t)\rho$ of the same form but with the substitution $M_{2k}^{s_{2k}, s'_{2k}} M_{2k+1}^{s_{2k+1}, s'_{2k+1}} \rightarrow M_{2k,2k+1}^{s_{2k}, s_{2k+1}, s'_{2k}, s'_{2k+1}}$. Now we find the optimal operator ρ_L, which has the form of Eq. (2), and is built from matrices of fixed dimension. As before, by optimal we mean that the distance to the original one is minimized. This time we use as a measure of the distance $E_{\rm HS}(\rho_o, \rho_L)$ and thus we do not impose the condition (3) (the use of E_F in this context is more complicated and will be explored in a future work). This leads to an optimization algorithm which is very much like the one introduced before at the level of purification, but in which now ρ_o and ρ_L are treated as vectors on a $\mathbf{d}^N$-dimensional space, where $\mathbf{d} = d \times d$. This way, it is possible to use the same code for studying the evolution of both pure and mixed states. We note that, while this method cannot guarantee the positivity of the truncated operator $\rho_L(t)$ obtained at the end of the algorithm, if the truncation error $E_{\rm HS}(\rho_o, \rho_L)$ is kept small, it will be possible to bound the errors made when using $\rho_L(t)$ to compute expectation values of any physical quantity. Note also that the matrices $M_k^{s_k, s'_k} \in \mathbb{C}^{L_k \times L_k}$ do not need to have a size $L_k = D_k^2$ (which is the square of a number).

As an illustration, we have simulated the decay of correlations of the Greenberger-Horne-Zeilinger state $|\psi(0)\rangle = (1/\sqrt{2})(|0\rangle^{\otimes N} + |1\rangle^{\otimes N})$ and of a cluster state [20], under the evolution dictated by Eq. (9). In Fig. 2(a) we show the errors for simulations with up to $N = 8$ spins, a size for which we can compute the solution numerically with direct methods (a Crank-Nicholson

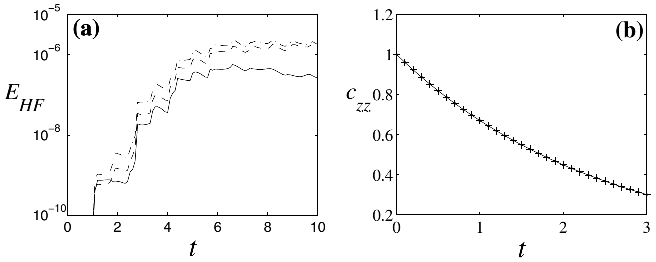

FIG. 2. (a) Errors in simulations of a cluster state with $N = 6$, 7, and 8 spins (solid line, dashed line, and dash-dotted line), under Eq. (9), for $\gamma = 0.1$, $h = 0$, matrices of size $L = 14$ and time step $\Delta t = 0.01$. (b) Decay of correlations, $c_{zz} = \langle\sigma_i^z\sigma_{i+1}^z\rangle - \langle\sigma_i^z\rangle\langle\sigma_{i+1}^z\rangle$, for the site $i = N/2$, on GHZ states with $N = 10$, 20, and 30 spins (dots, crosses, and solid line) for $L = 10$.

method which already has an error of the order of 10^{-10}). There are two sources of errors in our method. One is the Trotter expansion (10), but as it is of order $\mathcal{O}(\Delta t^2)$, it can be decreased by making shorter time steps. The second source of error is the truncation of the MPDO to a lower dimension. In the problems that we have simulated, truncation error affected only the cluster state and did not grow much with the size of the system. In Fig. 2(b) we plot some simulations made with GHZ states of up to 50 spins, from which an exponential decay law for the correlation functions, $c_{zz}(t) = \langle\sigma_i^z\sigma_{i+\Delta}^z\rangle - \langle\sigma_i^z\rangle\langle\sigma_{i+\Delta}^z\rangle \simeq e^{-4\gamma t}$, can be extracted. The method is rather efficient and can easily handle this and bigger problems in ordinary computers.

In summary, we have introduced the concept of matrix product density operators (MPDO) and their purification in terms of matrix product states (MPS) in order to describe mixed states in quantum many-body systems. We have also developed a method to determine the MPS (MPDO) which optimally describes another one which is composed of matrices of higher dimensions. We have used those ideas to introduce an algorithm which allows us to study 1D systems in thermal equilibrium. In contrast to previous methods, it applies to *finite* systems, with general long-range interactions (not necessarily translationally invariant) and works over the whole range of temperatures $T \in [0, \infty)$. In fact, the algorithm is a very natural extension of DMRG to finite temperatures because for $T \rightarrow 0$ one recovers the same MPS that one would obtain with standard DMRG. We have also shown how to simulate the evolution of a system in the presence of dissipation, i.e., when it evolves according to a master equation which involves short-range interactions. We note that in this last case an alternative possibility is to combine the concepts introduced here with the "quantum jump" approach [21]. The idea is to perform several realizations of the evolution starting out with randomly chosen pure states in such a way that their mixture reproduces the initial MPDO (2). In each realization the pure state is evolved according to a stochastic Schrödinger equation consisting of a time evolution with an effective Hamiltonian which is interrupted by quantum jumps [21]. After each short time step (or quantum jump) the new pure state is determined using the method introduced here and which optimally approximates the new state with a MPS. At the end, expectation values of physical observables are determined by averaging with respect to the different realizations. Which of these two methods is more efficient will depend on the number of realizations one has to perform in practice in the latter in order to achieve a prescribed accuracy.

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