Mixed-State Dynamics in One-Dimensional Quantum Lattice Systems: A Time-Dependent Superoperator Renormalization Algorithm

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We present an algorithm to study mixed-state dynamics in one-dimensional quantum lattice systems. The algorithm can be used, e.g., to construct thermal states or to simulate real time evolution given by a generic master equation. Its two main ingredients are (i) a *superoperator* renormalization scheme to efficiently describe the state of the system and (ii) the time evolving block decimation technique to efficiently update the state during a time evolution. The computational cost of a simulation increases significantly with the amount of correlations between subsystems, but it otherwise depends only linearly on the system size. We present simulations involving quantum spins and fermions in one spatial dimension.

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The most interesting quantum phenomena involve strongly correlated many-body systems, but studying such systems—a central task in the areas of condensed matter physics, quantum field theory, and, since recent years, also quantum information science [1,2]—has too often proven a formidable challenge. Indeed, in quantum many-body theory only a few exact solutions are available, while most analytical approximations remain uncontrolled. As a consequence, numerical calculations are of great importance. But even these suffer from a severe computational obstacle: an exponential growth of degrees of freedom with the system size that renders the direct simulation of most quantum systems prohibitively inefficient. And yet, ingenious methods such as quantum Monte Carlo techniques [3] can be used to approximately evaluate, e.g., certain ground state properties in quantum lattice models. In one-dimensional lattices, strikingly accurate results for quantities such as ground state energies and two-point correlators can be obtained by using White's *density matrix renormalization group* (DMRG) [4] technique, which has dominated most numerical research in the field since its invention more than a decade ago. Generalizations of the DMRG have also yielded accurate low energy spectra [5] or allowed for the simulation of real time evolution for small times [6].

Recently, the *time evolving block decimation* (TEBD) algorithm [7] has been proposed to simulate real time evolution in one-dimensional quantum lattice systems. This technique can be easily adapted into standard DMRG implementations [8,9] and seems to be very efficient [8–10]. As in DMRG, a decisive factor in the performance of the TEBD method is that not a lot of entanglement is present in the system, a condition that is ordinarily met in one-dimensional lattices at low energies [7].

In this Letter we extend the TEBD algorithm to handle mixed states. We describe how to efficiently simulate, in one-dimensional quantum lattice systems, real time Markovian dynamics as given by a (possibly time-dependent) master equation made of arbitrary nearest neighbor couplings. By considering evolution in imaginary time, the present extension can also be used to construct thermal states for any given temperature. Thus, we show how to numerically explore nonequilibrium many-body dynamics under realistic conditions, including the effects of finite temperature and decoherence.

A key observation for the success of the algorithm is that in one spatial dimension many states of interest, including thermal states and local perturbations thereof, contain only a restricted amount of correlations between subsystems, in a sense to be further specified. This fact allows us to introduce an efficient decomposition for the state of the system, referred to as *matrix product decomposition* (MPD). The MPD is a mixed-state version of a matrix product state [11], and, as such, we can use the TEBD to update it during a time evolution. It also follows that our scheme can again be fully incorporated into standard DMRG implementations without much programming effort [8,9].

We consider a generic one-dimensional quantum lattice made of n sites, labeled by index l, $l \in \{1, \ldots, n\}$, each one described by a local Hilbert space $\mathbb{H}^{[l]} \cong \mathbb{C}_d$ of finite dimension d. We assume the evolution of the n sites, in a global state ρ, is given by a master equation [2]

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

where H and L_μ are the Hamiltonian and Lindblad operators, and where we require that the (possibly time-dependent) Lindbladian superoperator $\mathcal{L}$ further decom-

poses into terms involving at most two contiguous sites,

$$\mathcal{L}[\rho] = \sum_l \mathcal{L}_{l,l+1}[\rho]. \tag{2}$$

Reduced superoperators.—A pure-state evolution is described by a vector $|\Psi\rangle$ in the n-fold tensor product of $\mathbb{C}_d$. Let us divide the n sites into two blocks, denoted L (left) and R (right). Then DMRG and TEBD consider reduced density matrices, e.g., that of block L [12],

$$|\Psi\rangle \in \mathbb{C}_d^{\otimes n} \to \rho^{[L]} \equiv \mathrm{tr}_R(|\Psi\rangle\langle\Psi|) \in \mathbb{L}(\mathbb{H}^{[L]}), \tag{3}$$

where $\mathbb{L}(\mathbb{H})$ denotes the set of linear mappings on $\mathbb{H}$ or, equivalently, the complex vector space of $\dim(\mathbb{H}) \times \dim(\mathbb{H})$ matrices. Here we are concerned with the evolution of a mixed state, which requires more notation. For each site l, let $\mathbb{K}^{[l]} \cong \mathbb{L}(\mathbb{H}^{[l]}) \cong \mathbb{C}_{d^2}$ denote the vector space of $d \times d$ complex matrices. We switch into representing a density matrix $\sigma \in \mathbb{L}(\mathbb{H})$ as a "superket" $|\sigma\rangle_\sharp \in \mathbb{K} \cong \mathbb{L}(\mathbb{H})$, while a superoperator $\mathcal{Q} \in \mathbb{L}(\mathbb{L}(\mathbb{H}))$ is regarded as a linear mapping $\mathcal{Q}_\sharp \in \mathbb{L}(\mathbb{K})$ [14],

$$\left.\begin{array}{c} |\Phi\rangle \in \mathbb{H} \\ \sigma \in \mathbb{L}(\mathbb{H}) \\ \mathcal{Q} \in \mathbb{L}(\mathbb{L}(\mathbb{H})) \end{array}\right\} \to \left\{\begin{array}{l} |\Phi\rangle_\sharp \in \mathbb{K}, \\ |\sigma\rangle_\sharp \in \mathbb{K}, \\ \mathcal{Q}_\sharp \in \mathbb{L}(\mathbb{K}), \end{array}\right. \tag{4}$$

where $|\Phi\rangle_\sharp \equiv ||\Phi\rangle\langle\Phi|\rangle_\sharp$. For $d \times d$ matrices A and B, the scalar product ${}_\sharp\langle|\rangle_\sharp$ between superkets $|A\rangle_\sharp$ and $|B\rangle_\sharp$, and the action of $\mathcal{Q}_\sharp$ on $|A\rangle_\sharp$, are defined through

$${}_\sharp\langle A|B\rangle_\sharp \equiv \frac{1}{d}\mathrm{tr}(A^\dagger B), \qquad \mathcal{Q}_\sharp|A\rangle_\sharp \equiv |\mathcal{Q}[A]\rangle_\sharp. \tag{5}$$

Also, if $\mathcal{Q}$ is a superoperator on a bipartite space $\mathbb{H}^{[L]} \otimes \mathbb{H}^{[R]}$ and $\{|M_\mu\rangle_\sharp\}$ is an orthonormal basis in $\mathbb{K}^{[R]} \cong \mathbb{L}(\mathbb{H}^{[R]})$, we define the partial trace of $\mathcal{Q}_\sharp$ over block R as

$$\mathrm{tr}_{\sharp R}(\mathcal{Q}_\sharp) \equiv \sum_\mu {}_\sharp\langle M_\mu|\mathcal{Q}_\sharp|M_\mu\rangle_\sharp. \tag{6}$$

Finally, let $\rho \in \mathbb{L}(\mathbb{C}_d^{\otimes n})$ be the state of the n-site lattice and $|\rho\rangle_\sharp$ its superket. We define the *reduced superoperator* for a block of sites, say, for block L, as

$$|\rho\rangle_\sharp \in (\mathbb{C}_{d^2})^{\otimes n} \to \mathcal{Q}_\sharp{}^{[L]} \equiv \mathrm{tr}_{\sharp R}(|\rho\rangle_\sharp\langle\rho|) \in \mathbb{L}(\mathbb{K}^{[L]}), \tag{7}$$

in analogy with (3), and rewrite Eq. (1) as

$$|\dot\rho\rangle_\sharp = \mathcal{L}_\sharp|\rho\rangle_\sharp, \tag{8}$$

which parallels the Schrödinger equation $|\dot\Psi\rangle = -iH|\Psi\rangle$.

Renormalization of reduced superoperators.—Given blocks L and R, the Schmidt decomposition of $|\rho\rangle_\sharp$ reads

$$\begin{aligned} |\rho\rangle_\sharp &= \sum_{\alpha=1}^{\chi_\sharp} \lambda_{\sharp\alpha}|M_\alpha^{[L]}\rangle_\sharp \otimes |M_\alpha^{[R]}\rangle_\sharp, \\ \lambda_{\sharp\alpha} &\geq \lambda_{\sharp\alpha+1} \geq 0, \end{aligned} \tag{9}$$

where the Schmidt superkets $\{|M_\alpha^{[L,R]}\rangle_\sharp\}$ fulfill

$$\begin{aligned} \mathcal{Q}_\sharp{}^{[L]}|M_\alpha^{[L]}\rangle_\sharp &= (\lambda_{\sharp\alpha})^2|M_\alpha^{[L]}\rangle_\sharp, \\ \mathcal{Q}_\sharp{}^{[L]} &\equiv \mathrm{tr}_{\sharp R}(|\rho\rangle_\sharp\langle\rho|), \end{aligned} \tag{10}$$

$$\begin{aligned} \mathcal{Q}_\sharp{}^{[R]}|M_\alpha^{[R]}\rangle_\sharp &= (\lambda_{\sharp\alpha})^2|M_\alpha^{[R]}\rangle_\sharp, \\ \mathcal{Q}_\sharp{}^{[R]} &\equiv \mathrm{tr}_{\sharp L}(|\rho\rangle_\sharp\langle\rho|). \end{aligned} \tag{11}$$

The rank $\chi_\sharp$ of the reduced superoperators $\mathcal{Q}_\sharp{}^{[L]}$ and $\mathcal{Q}_\sharp{}^{[R]}$ measures the amount of correlations between blocks L and R [13]. In principle its value is only bounded above by the dimensions of $\mathbb{K}^{[L]}$ and $\mathbb{K}^{[R]}$, which grow exponentially in the number of sites. However, as the examples below illustrate, many situations of interest involving one-dimensional mixed-state dynamics are only *slightly correlated,* in that the coefficients $\{\lambda_{\sharp\alpha}\}$ *decay very fast with* α. That is, a good approximation to $|\rho\rangle_\sharp$ can be obtained by truncating (9) so that only a relatively small number of terms are considered. Thus, whereas DMRG and TEBD are based on decimating the block space $\mathbb{H}^{[L]}$ supporting the reduced density matrix $\rho^{[L]}$ of pure-state $|\Psi\rangle$, Eq. (3), here we propose to decimate the block space $\mathbb{K}^{[L]} \cong \mathbb{L}(\mathbb{H}^{[L]})$ supporting the reduced superoperator $\mathcal{Q}^{[L]}$ in (7).

Matrix product decomposition and TEBD.—We regard ρ as a vector $|\rho\rangle_\sharp$ in the n-fold tensor product of $\mathbb{C}_{d^2}$, while the master Eq. (8) is formally equivalent to the Schrödinger equation. Mixed-state dynamics can therefore be simulated by adapting the pure-state techniques of [7]. Given an orthonormal basis $\{|i_l\rangle_\sharp\}$ of $\mathbb{K}^{[l]}$ for site l, we expand $|\rho\rangle_\sharp$ as

$$|\rho\rangle_\sharp = \sum_{i_1=0}^{d^2-1} \cdots \sum_{i_n=0}^{d^2-1} c_{i_1\cdots i_n}|i_1\rangle_\sharp \otimes \cdots \otimes |i_n\rangle_\sharp. \tag{12}$$

We choose $|0_l\rangle_\sharp = |I/d\rangle_\sharp$ to be proportional to the identity in $\mathbb{H}^{[l]}$, so that physical normalization of ρ, $\mathrm{tr}(\rho) = 1$, corresponds to $c_{0\cdots0} = 1$. Then we use a MPD,

$$c_{i_1 i_2 \cdots i_n} = \sum_{\alpha_1,\ldots,\alpha_{n-1}} \Gamma_{\alpha_1}^{[1]i_1} \lambda_{\sharp\alpha_1}{}^{[1]} \Gamma_{\alpha_1\alpha_2}^{[2]i_2} \lambda_{\sharp\alpha_2}{}^{[2]} \Gamma_{\alpha_2\alpha_3}^{[3]i_3} \cdots \Gamma_{\alpha_{n-1}}^{[n]i_n}, \tag{13}$$

which can be built through a succession of Schmidt decompositions of $|\rho\rangle_\sharp$ (see [7] for details). Finally, we update tensors $\{\Gamma^{[l]}\}$ and $\{\lambda_\sharp{}^{[l]}\}$ during an evolution of the form (1) and (2) by using the TEBD algorithm [15].

Example 1: Thermal state.—The mixed state,

$$\rho_\beta \equiv \frac{e^{-\beta H}}{Z(\beta)} = \frac{1}{Z(\beta)}\sum_s e^{-\beta E_s}|E_s\rangle\langle E_s|, \tag{14}$$

where H is a nearest neighbor Hamiltonian, $\beta \equiv 1/kT$ is the inverse temperature, and $Z(\beta) \equiv \mathrm{tr}(e^{-\beta H})$ is the partition function, can be well represented by a MPD that we

build by simulating an imaginary time evolution from the completely mixed state,

$$|e^{-\beta H}\rangle_\sharp = \exp(-\beta \mathcal{T}_\sharp)|I\rangle_\sharp. \tag{15}$$

Here superket $|I\rangle_\sharp$ and superoperator $\mathcal{T}_\sharp$ correspond to

$$|I\rangle_\sharp = |I_1\rangle_\sharp \otimes \cdots \otimes |I_n\rangle_\sharp, \qquad \mathcal{T}[A] \equiv \tfrac{1}{2}(HA + AH). \tag{16}$$

Indeed, $\exp(-\beta\mathcal{T}_\sharp)$ can be Trotter expanded into transformations involving only two adjacent sites, and the MPD can therefore be updated using the TEBD. Notice that a single run of the simulation builds the thermal state $\rho_{\beta'}$ for any intermediate value of $\beta' \in [0, \beta]$. Figure 1 corresponds to thermal states for a quantum Ising model with transverse magnetic field,

$$H = \sum_{l=1}^{n-1} \sigma_l^x \otimes \sigma_{l+1}^x + \sum_{l=1}^{n} \sigma_l^z. \tag{17}$$

Example 2: Time-dependent master equation.—We consider a lattice of $n = 100$ sites loaded with $n/2$ fermions that evolve according to a Lindbladian

$$\mathcal{L}[\rho] = -i[H, \rho] + \gamma \sum_{l=1}^{n} \left(n_l \rho n_l - \frac{1}{2}\rho n_l^2 - \frac{1}{2} n_l^2 \rho \right), \tag{18}$$

$n_l \equiv a_l^\dagger a_l$, where the last term accounts for phase damping and the Hamiltonian part corresponds to hopping between adjacent sites and a time-dependent on-site energy,

$$H = -J \sum_{l=1}^{n-1} (a_l^\dagger a_{l+1} + \text{H.c.}) - \mu(t) \left(\sum_{l=1}^{n/2} n_l - \sum_{l=n/2+1}^{n} n_l \right), \tag{19}$$

where $\mu(t) \equiv \mu_0 [e^{-(t-t_0)/t_s} + 1]^{-1}$ introduces a bias μ_0 between the left and right halves of the lattice at $t = t_0$. Figure 2 shows the particle current

$$-2\,\text{Im}\langle a_{50}^\dagger(t) a_{51}(t)\rangle \tag{20}$$

as a result of switching on the bias.

Example 3: Unequal-time correlators.—For the above fermion system with no bias, $\mu(t) = 0$, and finite temperature, we finally consider the expectation value

$$\langle a_l^\dagger(t) a_1(0)\rangle = \text{tr}(a_l^\dagger \mathcal{E}_t[a_1 \rho]), \tag{21}$$

where $\mathcal{E}_t$ is the time evolution operator resulting from the master equation. Since the Lindbladian $\mathcal{L}$ is time independent, we can integrate the master Eq. (8) to obtain $\mathcal{E}_{t_\sharp} = \exp(\mathcal{L}_\sharp t)$. The simulation (see Fig. 4) is achieved as follows: (i) the initial state of the system, a thermal state with $\beta = 1/J$, is obtained by evolution in imaginary

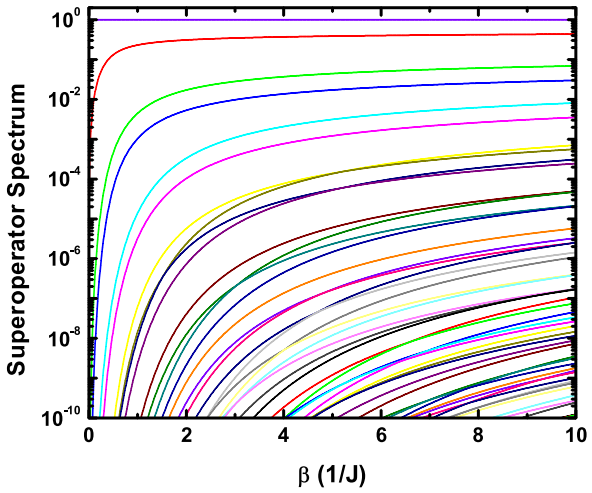

FIG. 1 (color online). Quantum Ising chain with transverse magnetic field, Eq. (17), at finite temperature. Local dimension $d = 2$, $n = 100$ sites, and effective $\chi_\sharp = 80$. At zero temperature, $\beta \to \infty$, this model corresponds to a quantum critical point. The spectrum $\{\lambda_{\sharp\alpha}{}^2\}$ of the reduced superoperator $\mathcal{Q}_\sharp{}^{[L]}$ for the left half chain is plotted as a function of $\beta \in [0, 10/J]$ (only the 52 largest eigenvalues are shown). For any inverse temperature β, a fast decay of $\lambda_{\sharp\alpha}{}^2$ in α ensures that the state can be accurately approximated by a MPD with small effective $\chi_\sharp$.

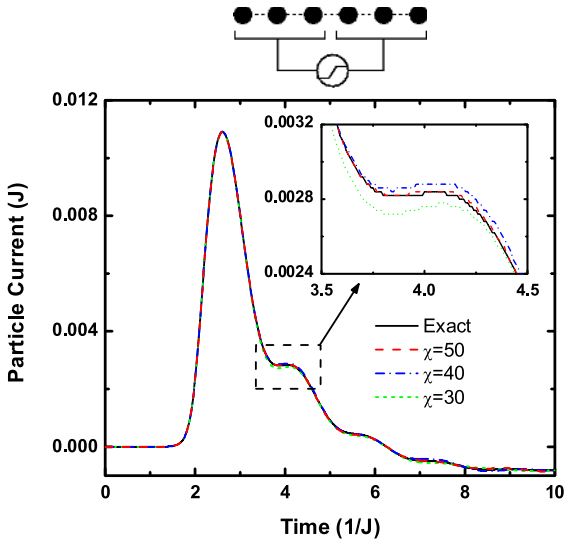

FIG. 2 (color online). Fermionic lattice of Eq. (18) at finite temperature $\beta = 1/J$, dephasing $\gamma = 0.4J$, bias $\mu_0 = 0.1J$, and with $d = 2$, $n = 100$. The particle current [see Eq. (20)] is due to a time-dependent applied bias $\mu(t)$ with turn-on time $t_0 = 2/J$ and rise time $t_s = 0.1/J$. The exact solution is obtained by numerically integrating the (Gaussian) time evolution for two-point correlators. Instead, the numerical simulations are achieved after mapping the fermion lattice into a spin lattice with nearest neighbor couplings by means of a Jordan-Wigner transformation. The time evolution is then broken into small gates for pairs of nearest neighbor spins and implemented using the TEBD algorithm. The simulations with an effective $\chi_\sharp = 30, 40, 50$ show rapid convergence to the exact solution. Figure 3 justifies such convergence. This will also be addressed in more detail in [13].

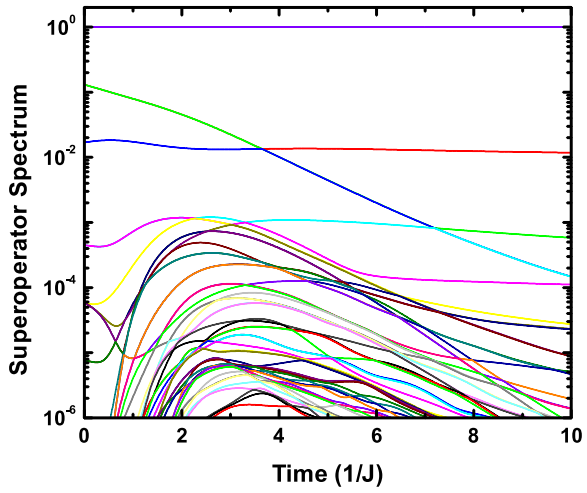

FIG. 3 (color online). Same system as in Fig. 2. The spectrum $\{\lambda_{\sharp\alpha}{}^2\}$ of the reduced superoperator $\mathcal{Q}_\sharp{}^{[L]}$ for the left $n/2$ sites is plotted as a function of time. The number of relevant eigenvalues $\lambda_{\sharp\alpha}{}^2$, say above 10^{-6}, increases as the applied bias is turned on, but remains small throughout the evolution, and it even decreases for long times.

time as explained in example 1; (ii) the annihilation operator a_1 is applied to the initial state ρ to obtain $a_1\rho$; (iii) $a_1\rho$ is evolved in time according to $\mathcal{E}_t$; (iv) the creation operator $a_l^\dagger$ is applied on $\mathcal{E}_t[a_1\rho]$; and (v) the trace of the resulting operator $a_l^\dagger\mathcal{E}_t[a_1\rho]$ is computed. Each of these steps can be performed efficiently by using a MPD and the update techniques of [7].

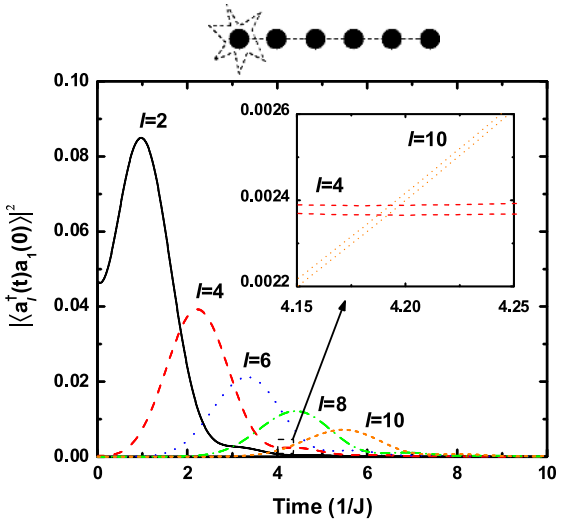

FIG. 4 (color online). Fermionic lattice of Eq. (18) at finite temperature $\beta = 1/J$, dephasing $\gamma = 0.4J$, and with $d = 2$, $n = 100$, and no applied bias, $\mu(t) = 0$. Unequal-time, two-point correlator (21) for $l = 2, 4, 6, 8, 10$ and $t \in [0, 10/J]$. The results corresponding to an effective $\chi_\sharp = 40$ and 50 practically overlap at all times, as the inset shows.

We have presented an extension of the TEBD algorithm to mixed states. With specific examples involving spins and noninteracting fermions, we have shown how to (i) construct thermal states; (ii) evolve a state in time according to a time-dependent master equation; and (iii) compute unequal-time correlation functions. The algorithm can be used for generic one-dimensional lattice systems, including interacting fermions and bosons [13]. See also Verstreate [16].

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[14] We use the subscript ♯ (sharp) to denote operators (superoperators) when represented as superkets (mappings between superkets).
[15] The evolution resulting from (8) is in general nonunitary in the space $(\mathbb{C}_{d^2})^{\otimes n}$ of superkets $|\rho\rangle_\sharp$. As explained in [13], the TEBD algorithm can still be used.
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