Renormalization algorithm with graph enhancement

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We introduce a class of variational states to describe quantum many-body systems. This class generalizes matrix product states which underlie the density-matrix renormalization-group approach by combining them with weighted graph states. States within this class may (i) possess arbitrarily long-ranged two-point correlations, (ii) exhibit an arbitrary degree of block entanglement entropy up to a volume law, (iii) be taken translationally invariant, while at the same time (iv) local properties and two-point correlations can be computed efficiently. This variational class of states can be thought of as being prepared from matrix product states, followed by commuting unitaries on arbitrary constituents, hence truly generalizing both matrix product and weighted graph states. We use this class of states to formulate a renormalization algorithm with graph enhancement and present numerical examples, demonstrating that improvements over density-matrix renormalization-group simulations can be achieved in the simulation of ground states and quantum algorithms. Further generalizations, e.g., to higher spatial dimensions, are outlined.

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I. INTRODUCTION

Strongly correlated quantum systems give rise to a number of intriguing phenomena in condensed-matter systems such as the existence of rare-earth magnetic insulators or high-temperature superconductors. The classical description or analytic solution of such quantum many-body systems is however difficult in general, as entanglement and interactions cannot be neglected and the dimension of the underlying Hilbert space grows exponential with the number of constituent particles. Nevertheless, a number of powerful classical simulation methods have been developed and successfully applied, including variational approaches such as, e.g., the *density-matrix renormalization group* (DMRG) [1,2] and their generalizations [3–5].

The key problem in such variational approaches is to identify families of states that show the relevant features of the system in question and which at the same time can be *efficiently* described and analyzed. DMRG can indeed be seen as the variation over the family of matrix product states (MPSs) [6–9] described by a polynomial number of parameters. The power and limitation of DMRG (and related methods) can be understood from the entanglement features of the MPSs, where, e.g., correlations decay exponentially and blockwise entanglement fulfills an area law [10]. Other families such as *weighted graph states* (WGSs) [11–13] can em-

body long-ranged correlations in any spatial dimension and blockwise entanglement scaling with the volume, as is, e.g., the case for time evolution [14] but do not seem to grasp short-range properties as well as MPSs do [15].

Given the complementary strength of MPS and WGS, it seems natural to attempt a unification of the two approaches. Here we show that this is indeed possible; i.e., we describe a variational method based on a family of states which combines the favorable features of MPS and WGS while maintaining the possibility to efficiently calculate local properties and correlation functions. We demonstrate the applicability and performance as well as limitations of the new method for ground-state approximation. The relevance of this unification is however not only limited to ground-state approximation but can also be employed to simulate time evolution and certain kinds of quantum computations. In fact, we demonstrate that the method is suited to simulate certain quantum circuits and algorithms, which in turn leads to classical algorithms for the corresponding problems.

On a more fundamental level, we contribute toward an improved understanding of the border line between the classical and the quantum. In particular, our results give insights on the responsible features of quantum mechanics that make quantum computers potentially more powerful than classical devices and on the conditions under which an efficient classical simulation of quantum systems is possible. It turns out

that small (blockwise) entanglement (as in MPS), the sole usage of commuting operations (as for WGS), or special gate sets (Clifford circuits) are not necessary to guarantee an efficient classical simulation. In fact, the family of states we introduce allows us to continuously interpolate between these extreme cases.

This paper has the following structure. In Sec. II, we discuss the renormalization algorithm with graph enhancement (RAGE) class of variational states and investigate their properties and relations to matrix product states and graph states. In Sec. III, we show how to compute reduced density matrices—the fundamental object for the evaluation of expectation values of local operators—of this state class efficiently. In Sec. IV, we show how to update the parameters of the RAGE states in order to minimize ground-state energies and to maximize overlaps in a time evolution algorithm. Besides stating the algorithmical principle, the (numerical) results of applications to example problems are given. In Secs. V and VI, we discuss possible generalizations of the RAGE class and conclude this paper.

II. RENORMALIZATION ALGORITHM WITH GRAPH ENHANCEMENT

We start from MPS of a quantum chain of length N, consisting of d-level systems, as used in DMRG [6–9],

$$|\psi(A)\rangle := \sum_{s_1,\ldots,s_N=0}^{d-1} \mathrm{tr}[A_{s_1}^{(1)}\cdots A_{s_N}^{(N)}]|s_1,\ldots,s_N\rangle, \qquad (1)$$

where the $A_{s_n}^{(n)}$ are complex $D \times D$ matrices. For open boundary conditions, the leftmost and rightmost matrices can be taken to be vectors. For simplicity of notation, but in a way that can be trivially generalized, we now fix $d=2$. MPSs have correlation functions

$$\langle Z^{(j)}Z^{(j+k)}\rangle - \langle Z^{(j)}\rangle\langle Z^{(j+k)}\rangle,$$

exponentially decaying in k and satisfy an area law [10] by construction [16]. An area law in one dimension implies that any Renyi entropy S_α of the reduced state of a block of L contiguous spins will eventually saturate [$S_\alpha(\rho_L)=O(1)$]; many ground states possess this property and hence a good and economical MPS approximation of them is possible [17].

Now we go beyond this picture and apply to the MPS any set of commuting unitaries between any two constituents, irrespective of the distance. More specifically, we consider the adjacency matrix Φ of a weighted simple graph with $\Phi_{k,l} \in [0,2\pi)$ and apply without loss of generality the corresponding *phase gates*,

$$U(\Phi_{k,l}) := |0,0\rangle\langle0,0| + |0,1\rangle\langle0,1| + |1,0\rangle\langle1,0|$$
$$+ |1,1\rangle\langle1,1|e^{i\Phi_{k,l}}, \qquad (2)$$

between the particles k,l in the chain. Finally, we apply local rotations $V_j \in U(2)$ to arrive at the variational class of states defined by

$$|\psi(\Lambda,\Phi,V)\rangle := \prod_{j=1}^{N} V_j^{(j)}\prod_{k,l} U^{(k,l)}(\Phi_{k,l}) \sum_{s_1,\ldots,s_N} \mathrm{tr}[A_{s_1}^{(1)}\cdots A_{s_N}^{(N)}]$$
$$\times |s_1,\ldots,s_N\rangle, \qquad (3)$$

which then forms the basis of the RAGE.

A. Relationship with matrix product and weighted graph states

The above set clearly embodies a large variational class. By definition, for $\Phi=0$ and $V_j=1$, it includes the MPS. It also includes superpositions of WGS as first considered in Ref. [13],

$$|\varphi\rangle = \sum_m \alpha_m \prod_{j=1}^{N} V_j^{(j)} \sum_{s_1,\ldots,s_N=0}^{1} e^{-is^T\Phi s + d_m^T s}|s_1,\ldots,s_N\rangle$$
$$= \prod_{j=1}^{N} V_j^{(j)}\prod_{k,l} U^{(k,l)}(\Phi_{k,l}) \sum_m \alpha_m|\eta_{m,1}\rangle \otimes \cdots \otimes |\eta_{m,N}\rangle, \qquad (4)$$

where $\mathbf{d}_m=(d_{m,1},\ldots,d_{m,N})$, $\mathbf{s}=(s_1,\ldots,s_N)$, $|\eta_{m,n}\rangle:=|0\rangle + e^{d_{m,n}}|1\rangle$, and $U(\Phi_{m,n})$ are defined as above and which can be shown to be of the form of Eq. (3). For simplicity and without loss of generality, we will often set $V_j=1$ subsequently.

B. Main properties of RAGE states

To start with, RAGE states have a polynomially sized description, where the MPS and the WGS parts are fully determined by $O(ND^2)$ and $O(N^2)$ real parameters, respectively.

(i) *Volume law for the entanglement entropy.* By having a collection of maximally entangled qubit pairs across a boundary, the von Neumann entropy of a block of size L can be taken to scale as $S(\rho_L)=O(L)$. Encompassing graph states, our class can hence maximize the entanglement entropy.

(ii) *Translational invariance.* Whenever the MPS part is translationally invariant, Φ is a cyclic matrix and V_j is the same for all j, the whole state $|\varphi\rangle$ is manifestly translationally invariant. There exist other translationally invariant states that do not have this simple form. The key feature, though, is that unlike for multiscale entanglement renormalization [3], there exists this natural subset of states for which translational invariance is guaranteed to be exactly fulfilled, while at the same time a volume law for blockwise entanglement is possible [11,12].

(iii) *Completeness.* As MPSs already form a complete set in Hilbert space [if one allows D to scale as $O(2^N)$, one can represent any pure state in $(\mathbb{C}^2)^{\otimes N}$] and this remains true for the RAGE set.

III. EFFICIENT COMPUTATION OF LOCAL PROPERTIES AND CORRELATION FUNCTIONS

The previous properties are all very natural and desirable and especially (i) cannot be achieved efficiently with MPS alone. However, as will be shown, this does not prevent us

from computing local properties and correlation functions efficiently—which is the key feature of this set.

To compute expectation values of observables with small support we use the relevant reduced density matrix ρ_S, which may be computed efficiently with an effort of $O(ND^5)$ in the total size N of the system $S \subset \{1, \ldots, N\}$. Controlled phase gates acting exclusively on qubits that are traced out make no contribution. We define

$$E_{k,l}^{(j)} := \Lambda_k^{(j)} \otimes (\Lambda_l^{(j)})^*,$$

where $*$ denotes complex conjugation. The reduced density matrix ρ_S (up to phase gates in S) is then found to be

$$\rho_S = \sum_{\substack{s_1, \ldots, s_N = 0 \\ r_1, \ldots, r_N = 0}}^{1} \text{tr}[E_{s_1, r_1}^{(1)} \cdots E_{s_N, r_N}^{(N)}] \text{tr}_{\overline{S}}\left[\left(\prod_{k,l} U^{(k,l)}(\omega_{k,l})\right)\right.$$
$$\left. \times |s_1, \ldots, s_N\rangle\langle r_1, \ldots, r_N| \left(\prod_{k,l} U^{(k,l)\dagger}(\omega_{k,l})\right)\right]$$
$$= \sum_{\substack{s_1, \ldots, s_N = 0 \\ r_1, \ldots, r_N = 0}}^{1} \text{tr}[E_{s_1, r_1}^{(1)} \cdots E_{s_N, r_N}^{(N)}]|s_{m_1}, \ldots, s_{m_{|S|}}\rangle$$
$$\times \langle r_{m_1}, \ldots, r_{m_{|S|}}| \prod_{k \in S, l \in \overline{S}} e^{2i\Phi_{k,l}(\delta_{s_k,1} - \delta_{r_k,1})\delta_{s_l,1}}$$
$$\times \prod_{k \in S, l \in S} e^{i\Phi_{k,l}(\delta_{s_k,1} - \delta_{r_k,1})\delta_{s_l,1}} \prod_{s_i, r_i \in \overline{S}} \delta_{s_i, r_i}.$$

The key of the above argument is that the effect of the phases is a mere modification of the transfer operators of the MPS by a phase factor, the phase depending on the matrix element in question. Thus, the evaluation of expectation values is performed using (products of) transfer operators associated with the single sites. The reduced state can then be written as

$$\rho_S = \sum_{\substack{s_{m_1}, \ldots, s_{m_{|S|}} = 0 \\ r_{m_1}, \ldots, r_{m_{|S|}} = 0}}^{1} \text{tr}\left[\prod_{k=1}^{N} T^{(k)}(\{s_{m_p}, r_{m_p} : m_p \in S\})\right]$$
$$\times |s_{m_1}, \ldots, s_{m_{|S|}}\rangle\langle r_{m_1}, \ldots, r_{m_{|S|}}|,$$

where now

$$T^{(k)}[(s_{m_p}, r_{m_p})] := \sum_{l=0}^{1} B_l^{(k)}[(s_{m_p})] \otimes \{B_l^{(k)}[(r_{m_p})]\}^*,$$

which are the transfer operators modified by phases,

$$B_l^{(k)}(\{s_{m_p}\}) := A_l^{(k)} \prod_{m_p \in S} e^{if\Phi_{m_p,k}\delta_{s_{m_p},1}\delta_{l,1}},$$

where $f = 1$ if $k \in S$ and $f = 2$ if $k \in \overline{S}$. Grouped in this way, the reduced density operator can indeed be evaluated efficiently. In fact, for each $\{r_{m_p}, s_{m_p}\}$ the effort to compute the entry of the reduced state is merely $O(ND^5)$, as one has to multiply N transfer matrices of dimension $D^2 \times D^2$, just as in the case of MPS. This procedure is inefficient in $|S|$ with an exponential scaling effort. However, any Hamiltonian with

two-body (possibly long-ranged) interactions can be treated efficiently term by term.

IV. EFFICIENT UPDATES

Besides procedures for the efficient computation of reduced density matrices and therefore expectation values, we need a variational principle to improve the trial states. We will focus on local variational approaches to approximate ground states by minimizing the energy,

$$E := \frac{\langle\psi(A, \Phi, V)|H|\psi(A, \Phi, V)\rangle}{\langle\psi(A, \Phi, V)|\psi(A, \Phi, V)\rangle}, \tag{5}$$

on the approximation of time evolution and on the simulation of quantum circuits. The search for ground states is well known to be related to imaginary-time evolution.

A. Static updates

The MPS part can be updated as in variants of DMRG [9]. The expression $\langle\psi(A, \Phi, V)|H|\psi(A, \Phi, V)\rangle$ is (as in MPS) a quadratic form in each of the entries of the matrices $A_0^{(k)}, A_1^{(k)}$ for each site $k = 1, \ldots, N$. An optimal local update can therefore be found by means of solving generalized eigenvalue problems with an effort of $O(D^3)$. Local rotations can be incorporated by parametrizing single-qubit rotations on spin k with a normalized vector $\boldsymbol{x}_k \in \mathbb{R}^4$ as

$$V_k = x_{k,0}\mathbb{1} + i(x_{k,1}\sigma_x - x_{k,2}\sigma_y + x_{k,3}\sigma_z).$$

Again, the local variation in $\boldsymbol{x}_k$ in Eq. (5) is a generalized eigenvalue problem in $\boldsymbol{x}_k$ for each site $k = 1, \ldots, N$. To optimize the phases of the WGS, one may first define the Hamiltonian,

$$H_V := \left(\prod_{j=1}^{N} V_j^{(j)\dagger}\right) H \left(\prod_{k=1}^{N} V_k^{(k)}\right).$$

The optimal phase gates between any pair of spins $j, k \in \{1, \ldots, N\}$ can be computed efficiently as the procedure amounts to a quadratic function of a single variable $z = e^{i\Phi_{j,k}}$. To summarize, an update of $|\psi(A, \Phi, V)\rangle$ to minimize Eq. (5) corresponds to a sweeping over such local variations, each of which is efficiently possible, with an effort of $O(MND^3)$ for M sweeps. An element that is not present for MPS alone is that one can make a choice whether one adapts an MPS part or the adjacency matrix for an identical change in the physical state. In practice, we have supplemented this procedure with a gradient-based global optimization, making use of the fact that the gradient can be explicitly computed.

We have applied the RAGE method to proof-of-principle one-dimensional (1D) and two-dimensional (2D) models, where the adjacency matrix is allowed to connect any constituents in the lattice. Figure 1 shows the results for the 2D Ising model with transversal magnetic field,

$$H = J\sum_{\langle a,b\rangle} \sigma_z^{(a)}\sigma_z^{(b)} + B\sum_a \sigma_x^{(a)},$$

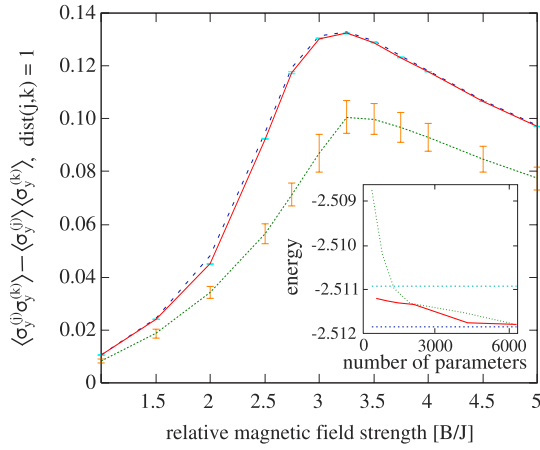comparing the achievable accuracy of MPS (using a one-dimensional path in the 2D lattice) and the RAGE method

FIG. 1. (Color online) 2D Ising model on a 4×4 periodic lattice. We compare the achievable accuracy with RAGE (red, solid) and MPS (green, dotted) with $D=4$ with exact results (blue, dashed). The total numbers of independent parameters are 384 for MPS and 552 for the RAGE state. Two-point correlations as a function of B are shown. The inset depicts the energy for different *total* numbers of parameters and $B=2$ in comparison with the exact ground state (blue, dashed) as well as the first-excited state (light blue, dashed).

for a fixed total number of free parameters. The RAGE method gives a significantly better accuracy regarding ground-state energy and two-point correlations, already for a very small number of parameters.

This class of states does allow for new features such as long-range correlations and a violation of an area law but, in turn, breaks the local SU(2) gauge invariance. It is also clear
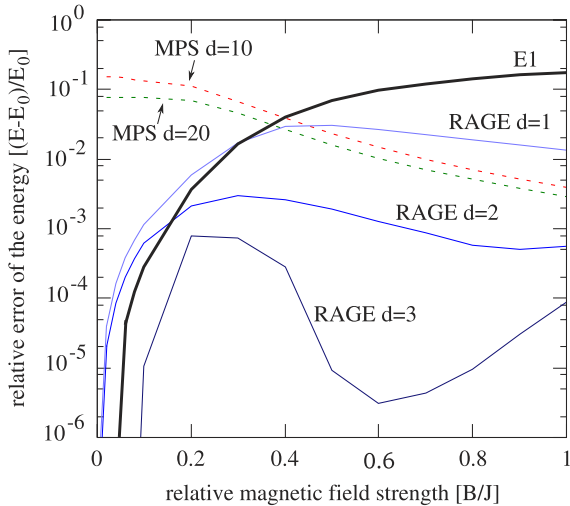

FIG. 2. (Color online) Kitaev model on a periodic 2D lattice with $N=12$ with magnetic field B in x direction. We compare the achievable accuracy for the ground state with MPS ($D=20$ and $D=10$) (broken lines) and RAGE with fixed phases and underlying MPS of $D=1,2,3$ (solid thin lines), where $D=1$ corresponds to WGS. For $B=0$, the ground state is exactly described by a WGS. For comparison, the first-excited state is plotted (solid bold line). For larger N, similar results are found, although the exact treatment was no longer possible.
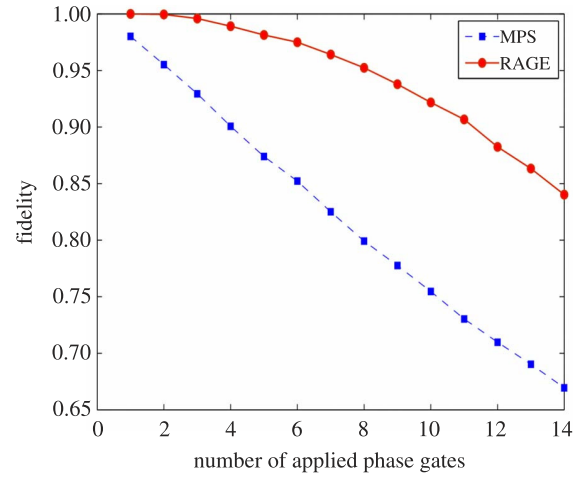

FIG. 3. (Color online) Comparison of MPS (blue, dashed) and RAGE (red, solid) with $D=2$ for the simulation of a random quantum circuit [19] on $N=14$ qubits. Application of a random local phase gate followed by a random controlled-phase gate with random uniform phase in $[0,2\pi)$ constitutes one block. For given k we apply this block k times to a randomly chosen initial MPS state. About 500 of such runs are determined, and in each the fidelity with the exact state is computed. The average over 500 realizations is then plotted.

from the simulations that the limitation of the underlying 1D structure of the MPS cannot always be fully overcome by the graph enhancement, as for certain models (e.g., for a 2D Heisenberg model) the overall accuracy is still not very satisfactory. The full potential in numerical performance in identifying ground states is yet to be explored.

However, the RAGE method is particularly well suited for certain interesting parent Hamiltonians. An example is the perturbed Kitaev model, whose ground state is, in the unperturbed case, the toric code state [18] and hence a graph state. We have considered Kitaev's model on a periodic 2D lattice where the additional perturbation was described by local magnetic fields (see Fig. 2). Even for fixed phases of the WGS—adjusted to match the toric code state at zero field—and an underlying MPS with $D=3$, we obtain a significantly improved accuracy as compared to WGS and MPS with a much higher number of parameters ($D=20$).

B. Time evolution and simulation of quantum circuits

We have also considered time evolution, more specifically the evolution of a quantum state in a quantum circuit. Here, sequences of elementary gates are applied, e.g., two-qubit phase gates and arbitrary single-qubit rotations. This method can be easily adapted to Hamiltonian (real or imaginary) time evolution. We now show how to efficiently obtain an optimal approximation of the resulting state after the application of an elementary gate. It turns out to be useful to restrict the variational family by setting $V_j^{(j)}=1$, although an extension to arbitrary V is possible. For phase gates, this update is particularly simple, as only a change in the adjacency matrix Φ is required. It is part of the strength of the scheme that phase gates between arbitrary constituents are

already included in the variational set. The update of a local unitary will require some more attention.

Consider an initial-state vector $|\psi(A,\Phi,\mathbb{1})\rangle$, to which a single-qubit unitary operation U is applied—acting, e.g., on the first qubit. The goal is now to find the best approximation $|\psi(A',\Phi',\mathbb{1})\rangle$ which maximizes

$$O := \frac{|\langle\psi(A',\Phi',\mathbb{1})|U_1|\psi(A,\Phi,\mathbb{1})\rangle|^2}{\langle\psi(A',\Phi',\mathbb{1})|\psi(A',\Phi',\mathbb{1})\rangle}. \quad (6)$$

It appears natural to vary only phases that directly affect qubit 1, i.e., $\Phi'_{j,k}=\Phi_{j,k}$ if $j \neq 1$. In this case, one can rewrite Eq. (6) in such a way that the optimal MPS part A' can be obtained analytically by solving a set of linear equations, while the optimization of a single phase $\Phi'_{1,k}$ leads to a simple quadratic form. In practice, an alternating sweeping of both kinds of local variational methods is required. We have tested this method for a random quantum circuit (see Fig. 3) and compared the achievable accuracy with MPS. Again, we obtain an improvement due to the WGS.

V. EXTENSIONS

A similar construction as illustrated for MPS also works for unifying WGS with other underlying tensor network descriptions. Similarly, one can use arbitrary Clifford circuits instead of the WGS, thereby generalizing the Gottesman-Knill theorem to simulate certain quantum circuits. More precisely, whenever an exact or approximate evaluation of expectation values of arbitrary product observables (i.e., tensor products of local operators) for a state described by a tensor network is possible, then *local* observables (i.e., observables with a small support) can be efficiently computed for the unified family of such tensor network states and WGS (or Clifford circuits), following an approach similar as in Eq. (4). While this certainly restricts the set of computable quantities (e.g., string-order parameters can no longer be evalu-ated), it still suffices to compute expectation values of all local Hamiltonians and hence one obtains a variational method for a ground-state approximation or simulation of quantum circuits.

VI. CONCLUSIONS

To summarize, we have discussed a variational class of states to describe quantum many-body systems. These states have a number of desirable properties. Correlation functions can be computed efficiently; systematic improvements of the approximation within the class are possible and the states carry long-range correlations and violate entanglement area laws, as being encountered in critical systems or in quenched quantum systems undergoing time evolution. We have applied the RAGE ansatz to condensed-matter and quantum computation problems, where we find an improvement over MPS. From a fundamental perspective the key question is where exactly the boundaries for the efficient classical description of quantum systems might lie. In fact, intriguingly, the entanglement content of the state cannot be taken as an indicator for the "complexity of a state" [20]. Delineating this boundary will reveal more about the structure of quantum mechanics from a complexity point of view and hold the potential for new improved algorithms and methods for the description of quantum systems.

ACKNOWLEDGMENTS

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