Simulation of Quantum Many-Body Systems with Strings of Operators and Monte Carlo Tensor Contractions

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We introduce string-bond states, a class of states obtained by placing strings of operators on a lattice, which encompasses the relevant states in quantum information. For string-bond states, expectation values of local observables can be computed efficiently using Monte Carlo sampling, making them suitable for a variational algorithm which extends the density matrix renormalization group to higher dimensional and irregular systems. Numerical results demonstrate the applicability of these states to the simulation of many-body systems.

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Introduction.—Explaining the properties of quantum many-body systems is a central topic in modern physics. Its difficulty is closely related to the hardness of finding a practical description of the quantum state of those systems. Therefore, results are usually derived by using either analytic approximations or numerical methods, as quantum Monte Carlo (QMC) [1] or the density matrix renormalization group (DMRG) [2]. While DMRG works extremely well for one-dimensional systems, Monte Carlo calculations proved very successful also in describing the behavior of nonfrustrated systems in higher dimensions. Recently, an extension of DMRG to two-dimensional systems has been developed which gives good results even for frustrated systems and time evolution [3–5]. It is based on projected entangled pair states (PEPS) which describe nature at low temperatures very well as has been proven by Hastings [6,7]. However, the class of states is too large [8], leading to an unfavorable scaling of the method in more than two dimensions or for periodic boundary conditions (PBC). Moreover, the algorithm relies on the underlying lattice structure so that irregular systems cannot be handled in a simple way. A subclass of PEPS which can be dealt with in an efficient way while keeping the power of the full family may be a solution to these issues.

In this Letter, we introduce a new class of states called *string-bond states*. String-bond states form a subclass of PEPS which contains the relevant states in quantum information, as, e.g., the toric code or the cluster state. Since expectation values can be computed easily on string-bond states using Monte Carlo sampling, they can be used to build a variational Monte Carlo algorithm for finding ground states. The central idea is to create the states by placing strings of operators on a lattice, which naturally extends the class of matrix product states (MPS) underlying DMRG to arbitrary geometries. Thus, the method combines the strengths of DMRG/PEPS and Monte Carlo: it can be applied to three-dimensional systems, systems with periodic boundary conditions, or general geometries by adapting the string pattern, but it also works for frustrated or fermionic systems which cannot be dealt with using QMC. At the same time, the computational resources scale favorably in the relevant parameters. We have implemented the method and successfully demonstrated its applicability.

String-bond states.—Consider a classical spin system with configurations $n=(n_1,\ldots,n_N)\in\{1,\ldots,d\}^N$ equipped with a probability distribution $p(n)$, and an efficiently computable function $f(n)$. The expectation value of $f(n)$, $\sum_n p(n)f(n)$, can be computed using Monte Carlo sampling—this is, by randomly sampling $f(n)$ according to the distribution $p(n)$—whenever $p(n)$ can be computed efficiently up to normalization. Turning towards quantum systems, for a state $|\psi\rangle$ and an observable O

$$\langle\psi|O|\psi\rangle=\sum_n\langle\psi|n\rangle\langle n|O|\psi\rangle=\sum_n p(n)\frac{\langle n|O|\psi\rangle}{\langle n|\psi\rangle} \quad (1)$$

with $p(n)=|\langle n|\psi\rangle|^2$, and therefore $\langle\psi|O|\psi\rangle$ can be evaluated using Monte Carlo whenever $\langle n|\psi\rangle$ and $\langle n|O|\psi\rangle$ can be computed efficiently. The latter reduces to $\langle\tilde{n}|\psi\rangle$ whenever $O=\sum D_k P_k$ with D_k diagonal and P_k permutations. In particular, this holds for local O (local meaning small support, as, e.g., two-point correlations) and products of Paulis, as, e.g., string order parameters.

To build a variational Monte Carlo method, one therefore has to construct states for which $\langle n|\psi\rangle$ can be computed efficiently. One such class is given by matrix product states (MPS) [9], the class of states underlying DMRG. An MPS with *bond dimension* D has the form

$$|\psi\rangle=\sum_{n_1,\ldots,n_N}\mathrm{Tr}[M^1_{n_1}\cdots M^n_{n_N}]|n_1,\ldots,n_N\rangle, \quad (2)$$

where each $M^i_{n_i}$ is a $D\times D$ matrix, so that $\langle n|\psi\rangle$ is given by the trace which can be computed efficiently. We generalize this to arbitrary geometries as follows.

Definition.—A state of N d-level spins is a string-bond state if there exists a local basis $|n\rangle=|n_1\rangle\cdots|n_N\rangle$ and a

set of strings $s \in \mathcal{S}$ (i.e., s is an ordered subset of $\{1, \ldots, N\}$) such that

$$\langle n|\psi\rangle = \prod_{s\in\mathcal{S}} \mathrm{Tr}\left[\prod_{x\in s} M^{s,x}_{n_x}\right] \tag{3}$$

for some complex $D \times D$ matrices $M^{s,n}_{n_x}$. Here, the product over $x \in s$ is over the sites x in the order in which they appear in the string.

Note that the trace of a product of operators in (3) resembles the structure of MPS (2). Some possible string arrangements are shown in Fig. 1.

The key point in the definition is the factorization of $\langle n|\psi\rangle$ into efficiently computable coefficients which we chose to be the trace of a matrix product. However, there are many more natural choices, as small "blobs" with, e.g., a PEPS parametrization or tree tensor networks [10]. A special case is given by quantum states corresponding to thermal states of classical models [11] which have strings between neighboring sites only, cf. Fig. 1(e).

A variational ansatz based on string-bond states generalizes DMRG beyond one-dimensional systems by combining it with Monte Carlo methods. In particular, due to the flexibility in the arrangement of the strings it can be adapted to arbitrary geometries, and the accuracy can be increased either by increasing D or by adding more strings. Clearly, the factorization of (3) does not imply that the string-bond states themselves factorize into matrix product states, and in fact they contain a large variety of relevant states.

Properties.—Let us first clarify the relation between string-bond states and projected entangled pair states (PEPS) [4]. To define a PEPS on any graph, place maximally entangled bonds $\sum_{i=0}^{D-1} |i\rangle|i\rangle$ on each edge—associating each virtual spin with one vertex—and apply a linear map $P^{[v]}$ on each vertex v which maps the virtual spins to the d-dimensional physical spin at v.

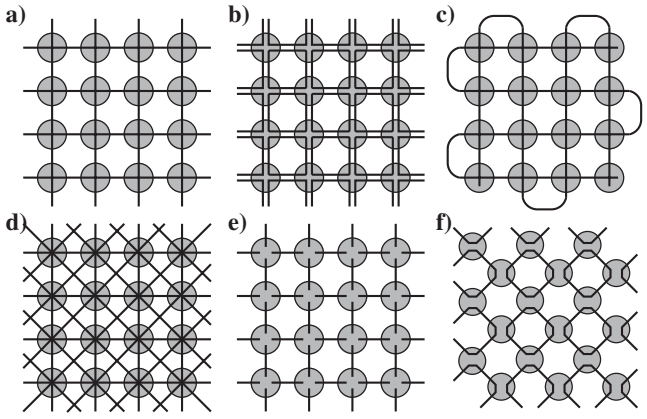

FIG. 1. Various string patterns. In (a), (c), and (d), the strings are long lines—in particular, (c) directly generalizes the DMRG ansatz, and since (d) contains (a), it gives a larger class of states. In (b) and (f), the strings form small loops; pattern (f) underlies the toric code state. In (e), the strings have length one, which suffices, e.g., for the cluster state or the coherent version of classical Gibbs states. Patterns (a), (b), and both atop of each other have been implemented numerically.

For clarity, we restrict to a 2D lattice with periodic boundaries. Consider a PEPS with linear maps

$$P^{[i,j]} = \sum_{s=0}^{d-1} |s\rangle\langle\phi^{a,s}_{i,j}|\langle\phi^{b,s}_{i,j}| \tag{4}$$

at site (i, j), where $\langle\phi^a|$ and $\langle\phi^b|$ act on two virtual spins each: one readily sees that together with the bonds they form strings [Fig. 2(a)], and $\langle n|\psi\rangle$ is given by the product of the overlaps of all strings. This generalizes the states corresponding to classical thermal states for which P factorizes completely [11]. On the other hand, every string-bond state can be written as a PEPS, even if at some edges many strings come to lie atop of each other. In that case, one places several maximally entangled bonds on that edge and uses one of them for each string. The product over the strings results in a factorizing map P as in (4), where the number of bipartite projectors $\langle\phi^{x,s}_{i,j}|$ equals the number of strings [see Fig. 2(b)]. Thus, the map pertains an efficient description, while the total bond dimension scales exponentially in the number of strings.

String-bond states are complete; i.e., every state can be written as a string-bond state for large enough D, even of form (4). This is easily seen by using one string which covers the whole system as in Fig. 1(c) and using the completeness of MPS [12].

String-bond states encompass a variety of relevant states in quantum information. First, this holds for all MPS as, e.g., the GHZ or the W state [12]. Any (generalized) weighted graph state, as, e.g., the cluster state [13], and thus all stabilizer states [14], are string-bond states with $D = 2$ [15]. The same is true for Kitaev's toric code state [16], using the pattern Fig. 1(f): the strings form loops, and the weight of each classical configuration is the parity of the four spins on the loop, corresponding to $P = |0\rangle\times\langle\psi^+|\langle\psi^+| + |1\rangle\langle\psi^-|\langle\psi^-|$ [11]. This results in a superposition of all states with an even number of $|1\rangle$'s on any loop, which is exactly the string condensate which gives the toric code state. In a sense, the string-bond states extend the

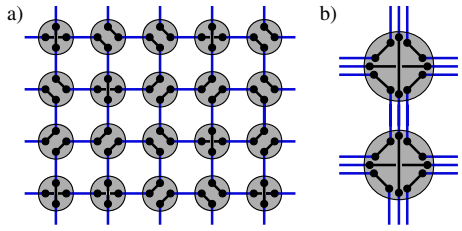

FIG. 2 (color online). (a) A PEPS with factorizing projectors—connected by the maximally entangled bonds (blue)—yields a string-bond state. (b) To convert a general string state with many strings [we illustrate patterns Fig. 1(a) and 1(b) together] into a PEPS, each string is routed over a separate bond.

construction of Kitaev [16] and Levin and Wen [17] and may help to add new insight into topological quantum computation. Note that both the cluster and the toric code state have a block entropy which scales as the area, and thus string states can achieve the entropic area law.

Variational ansatz.—The fact that expectation values of local observables and thus the energy of a local Hamiltonian H can be computed efficiently on string-bond states allows us to use them as a variational ansatz for the computation of ground state properties. Therefore, pick a string s, a site x on the string, and minimize the energy over the corresponding matrices $(M^{s,x}_{n_x})^d_{n_x=1} \equiv A$ (where A is a three-index tensor). By iterating this protocol until it converges, one gets a better and better approximation to the ground state.

For the optimization, we can use the linearity of string-bond states in A,

$$E(\psi_A) = \frac{\langle\psi_A|H|\psi_A\rangle}{\langle\psi_A|\psi_A\rangle} =: \frac{\langle \boldsymbol{A}|\boldsymbol{X}|\boldsymbol{A}\rangle}{\langle \boldsymbol{A}|\boldsymbol{Y}|\boldsymbol{A}\rangle}, \tag{5}$$

where we have explicitly denoted the dependence of the string-bond state $|\psi_A\rangle$ on A. $\langle \boldsymbol{A}|\boldsymbol{X}|\boldsymbol{A}\rangle$ denotes a quadratic form in A; i.e., $|\boldsymbol{A}\rangle$ is the vectorized form of A, where we use boldface to avoid confusion with vectors in state space. Minimizing (5) with respect to A is a generalized eigenvalue problem and can be solved efficiently.

However, solving the generalized eigenvalue problem requires a very high precision of $\boldsymbol{X}$ and $\boldsymbol{Y}$ and thus a very long Monte Carlo sample, rendering the approach infeasible. To overcome this problem, we use a Monte Carlo technique called *reweighting*. The idea is to replace the sampling over a distribution $p(n)$ by the sampling over some related distribution $p_0(n) \approx p(n)$,

$$\frac{\sum_n p(n) f(n)}{\sum_n p(n)} = \frac{\sum_n p_0(n) \frac{p(n)}{p_0(n)} f(n)}{\sum_n p_0(n) \frac{p(n)}{p_0(n)}}. \tag{6}$$

In our case, $p(n) = |\langle n|\psi_A\rangle|^2$, $p_0(n) = |\langle n|\psi_{A_0}\rangle|^2$ (where A_0 denotes the initial value of A), and $f(n) = \langle n|H|\psi_A\rangle/\langle n|\psi_A\rangle$, cf. Eq. (1). Now define $|\boldsymbol{a_n}\rangle$ and $|\boldsymbol{b_n}\rangle$ via the linear functionals

$$\langle \boldsymbol{a_n}|\boldsymbol{A}\rangle = \frac{\langle n|H|\psi_A\rangle}{\langle n|\psi_{A_0}\rangle}, \qquad \langle \boldsymbol{b_n}|\boldsymbol{A}\rangle = \frac{\langle n|\psi_A\rangle}{\langle n|\psi_{A_0}\rangle}. \tag{7}$$

Then one can readily check using (1) and (6) and that the matrices $\boldsymbol{X}$ and $\boldsymbol{Y}$ in (5) are

$$\boldsymbol{X} = \sum_n p_0(n) |\boldsymbol{b_n}\rangle\langle \boldsymbol{a_n}|, \qquad \boldsymbol{Y} = \sum_n p_0(n) |\boldsymbol{b_n}\rangle\langle \boldsymbol{b_n}|; \tag{8}$$

i.e., we can compute $\boldsymbol{X}$ and $\boldsymbol{Y}$ with a single Monte Carlo run.

The second problem is the inaccuracy of $\boldsymbol{X}$ and $\boldsymbol{Y}$ due to the finite sampling length: in particular, errors in the kernel of $\boldsymbol{Y}$ will very often lead to a wrong minimum. We overcome this problem by moving along the gradient of $E(\psi_A)$ by a small distance. With (5) and $\langle \boldsymbol{A}_0|\boldsymbol{Y}|\boldsymbol{A}_0\rangle = 1$, we find that

$$\text{grad}_A E(\psi_A)|_{A=A_0} = \boldsymbol{Y}|\boldsymbol{A}_0\rangle\langle \boldsymbol{A}_0|\boldsymbol{X}|\boldsymbol{A}_0\rangle - \boldsymbol{X}|\boldsymbol{A}_0\rangle \tag{9}$$

which only depends on absolute errors.

At this stage, we have an applicable algorithm. An extra speedup of (dD^2) is obtained by directly sampling the gradient: from (8) and (9) and $\langle \boldsymbol{b_n}|\boldsymbol{A}_0\rangle = 1$ [Eq. (7)],

$$\text{grad}_A E|_{A=A_0} = \sum_n p(n) |\boldsymbol{b_n}\rangle \left\{ \left[\sum_m p(m) h_m \right] - h_n \right\},$$

where we defined $h_n := \langle \boldsymbol{a_n}|\boldsymbol{A}_0\rangle = \langle n|H|\psi_{A_0}\rangle/\langle n|\psi_{A_0}\rangle$. Note that for local H, h_n only depends on the strings which intersect with H, and similarly $|\boldsymbol{b_n}\rangle$ only depends on the string which contains A. As h_n is independent of the site to be optimized, one can compute the gradients for *all* sites from the same sample and move along all of them simultaneously which gives another improvement of the order of the lattice size.

Numerical results.—In order to demonstrate the suitability of string-bond states for ground state calculations, we have implemented a simple nonoptimized MATLAB program for the string patterns Fig. 1(a) (lines) and Fig. 1(a) and 1(b) (lines + loops) on a 2D lattice with PBC. Adding loops typically leads to a significant improvement as it gives full control of correlations also to the first diagonal neighbor. Additional strings which supply connections to more diagonal neighbors further increase the accuracy.

We have tested our method by comparing it to the general PEPS algorithm [4,18], which is the only available general benchmark for frustrated systems. For the frustrated XX model on an 8×8 lattice with open boundary conditions (OBC), the general PEPS method gives $E = -92.39$ for $D = 4$, whereas string-bond states with lines + loops give $E = -93.31 \pm 0.02$ with $D = 8$, while at the same time being about 30 times faster. Apparently, the entanglement structure of frustrated systems is well reproduced only for large D, suggesting that string-bond states are very suitable to describe such systems due to their favorable scaling, and since they are not restricted to OBC. Figure 3 shows the magnetization for a frustrated XX model as a function of the transverse field for a 10×10 PBC lattice (computed with the lines + loops setup), for which we have no method to compare with.

To compare the algorithm for PBC, we have therefore investigated the 2D Ising model with transverse field and compared the results to quantum Monte Carlo (QMC) calculations [19]. Figure 4 shows the magnetization and the relative error in energy compared to QMC calculations as a function of the field. Already the two basic string setups used reproduce both energy and magnetization very well.

In all cases, we start with a very low number of sampling points, $M = 2000$, and with $D = 2$, and increase D or M or

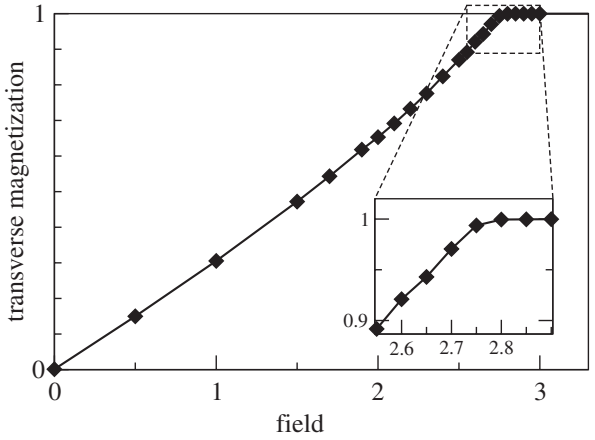

FIG. 3. Magnetization for a frustrated XX model (where each plaquette is frustrated) as a function of the transverse field on a 10×10 lattice with PBC. Note that there is no other method available which can deal with such systems.

refine the gradient step adaptively. Although for these values M the energy is very inaccurate, the gradient is still reliable, and the method typically converges after about 1000 iteration steps.

Outlook.—In this work, we have devised a class of states for which expectation values can be computed using Monte Carlo sampling, and which therefore can be used as a variational ansatz. The central idea is that for these states, $\langle n|\psi\rangle$ can be represented as a product of efficiently computable terms and in particular of matrix products.

The computation time scales as D^3 in the bond dimension (D^2 for open boundaries), which improves over the D^5 (D^3) scaling of DMRG. The reason is that the tensor network to be contracted has dimension D rather than D^2. For the same reason, Monte Carlo sampling can also be used to speed up the general PEPS method [4] from D^{10} to D^6.

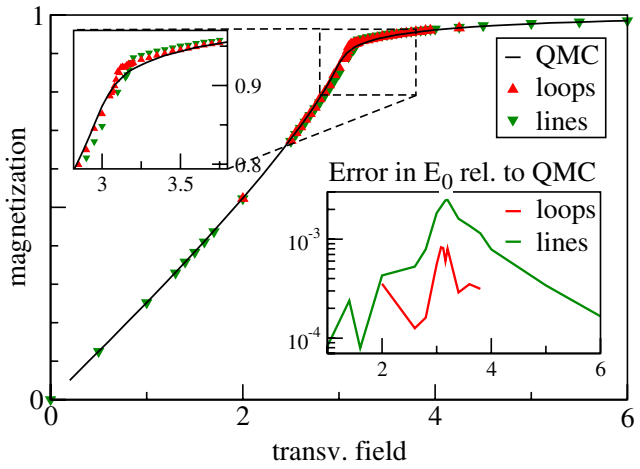

FIG. 4 (color online). Magnetization for the 10×10 PBC Ising model with transverse field: results for quantum Monte Carlo (QMC) and the string setups Fig. 1(a) (lines) and Fig. 1(a) and 1(b) (loops). The right inset shows the relative error in the ground state energy compared to QMC as a function of the field.

Several extensions to the ideas presented in this Letter are being investigated, for instance, different geometries for the factors of $\langle n|\psi\rangle$, the simulation of time evolutions or finite temperature systems as for DMRG, or the extension to fermionic systems, done either via a Jordan-Wigner transform (this leaves $\langle n|\psi\rangle$ computable) or using a fermionic ansatz for the variational Monte Carlo method.

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Note added.—The fact that Monte Carlo sampling can be used in tensor network contraction has been proposed independently in [20].

[1] W. von der Linden, Phys. Rep. **220**, 53 (1992).
[2] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005).
[3] G. Vidal, Phys. Rev. Lett. **93**, 040502 (2004).
[4] F. Verstraete and J. I. Cirac, arXiv:cond-mat/0407066.
[5] V. Murg, F. Verstraete, and J. I. Cirac, Phys. Rev. A **75**, 033605 (2007).
[6] M. B. Hastings, Phys. Rev. B **73**, 085115 (2006).
[7] M. B. Hastings, Phys. Rev. B **76**, 035114 (2007).
[8] N. Schuch, M. M. Wolf, F. Verstraete, and J. I. Cirac, Phys. Rev. Lett. **98**, 140506 (2007).
[9] A. Klümper, A. Schadschneider, and J. Zittartz, J. Phys. A **24**, L955 (1991); Z. Phys. B **87**, 281 (1992); M. Fannes, B. Nachtergaele, and R. F. Werner, Commun. Math. Phys. **144**, 443 (1992).
[10] M. Fannes, B. Nachtergaele, and R. F. Werner, J. Stat. Phys. **66**, 939 (1992); Y. Shi, L. Duan, and G. Vidal, Phys. Rev. A **74**, 022320 (2006).
[11] F. Verstraete, M. M. Wolf, D. Perez-Garcia, and J. I. Cirac, Phys. Rev. Lett. **96**, 220601 (2006).
[12] D. Perez-Garcia, F. Verstraete, M. M. Wolf, and J. I. Cirac, Quantum Inf. Comput. **7**, 401 (2007).
[13] S. Anders *et al.*, Phys. Rev. Lett. **97**, 107206 (2006).
[14] D. Schlingemann, Quantum Inf. Comput. **2**, 307 (2002).
[15] F. Verstraete and J. I. Cirac, Phys. Rev. A **70**, 060302 (2004).
[16] A. Kitaev, Ann. Phys. (Leipzig) **303**, 2 (2003).
[17] M. A. Levin and X.-G. Wen, Phys. Rev. B **71**, 045110 (2005).
[18] V. Murg (private communication).
[19] T. Roscilde (private communication).
[20] A. W. Sandvik and G. Vidal, Phys. Rev. Lett. **99**, 220602 (2007).