Matrix product states represent ground states faithfully

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We quantify how well matrix product states approximate exact ground states of one-dimensional quantum spin systems as a function of the number of spins and the entropy of blocks of spins. We also investigate the convex set of local reduced density operators of translational invariant systems. The results give a theoretical justification for the high accuracy of renormalization group algorithms and justifies their use even in the case of critical systems.

I. INTRODUCTION

Quantum spin systems show a very rich variety of fascinating phenomena. Despite the difficulty of describing such systems due to the large number of degrees of freedom, the development of both analytical and numerical techniques have allowed us to investigate and understand many of those phenomena. This success story is due, in part, to the discovery of renormalization group methods[1,2] which are very powerful scalable numerical techniques which seem to describe amazingly well the ground states of one-dimensional (1D) spin systems with local interactions in terms of matrix product states (MPSs).[3,4]

On the other hand, one may also investigate many-body quantum systems with a quantum computer or a quantum simulator.[5] For instance, one may use an adiabatic algorithm[6] to prepare the quantum simulator in the ground state of a prescribed Hamiltonian,[7] and then measure all one- and two-particle correlation functions. It seems that this approach may allow us to investigate the properties of many-body quantum systems that otherwise would not be describable by ordinary computers using existing numerical algorithms. In fact, an important effort is being made in order to build quantum simulators for some specific tasks.[8]

In this paper we present a series of analytical results which quantify the accuracy of the renormalization group methods. First, we give an expression that bounds the errors made by approximating general states of N spins by MPS in terms of the Renyi entropies corresponding to different subsystems. This result, when combined with the scaling of those Renyi entropies for critical 1D systems, implies that both short- and long-range properties of the low-energy states of critical spin chains can be very precisely described in terms of MPS with a number of parameters which only scales polynomially with N. This indicates that for those systems a quantum computer or simulator may not give us a big advantage with respect to a classical one. Second, we determine a bound on the error made in the approximation of two-particle reduced density operators coming from translationally invariant states in 1D by MPS in the limit $N \rightarrow \infty$. Finally, we illustrate the accuracy of renormalization group algorithms by some examples.

II. GROUND STATES AS CONVEX PROBLEMS

The determination of the ground state of a quantum system consisting of interacting spins on a lattice is highly nontrivial due to frustration effects. If one considers, e.g., a Heisenberg antiferromagnetic interaction between neighboring spins on a 1D spin chain, the energy would be minimized if all the reduced density operators of all neighboring spins would correspond to singlets. The monogamy properties of entanglement,[9–12] however, imply frustration effects which forbid the existence of such a state: if a particle A is maximally entangled with B, then it cannot be entangled with C. From the technical point of view, this can readily be proven by showing that the convex set of states obeying the semidefinite constraints $\rho_{ABC} \geq 0$; $\mathrm{Tr}_C(\rho_{ABC}) = |S\rangle\langle S| = \mathrm{Tr}_B(\rho_{ABC})$ with $|S\rangle = (|01\rangle - |10\rangle)/\sqrt{2}$ is empty. The frustration effects become stronger when the coordination number of the lattice increases.[9,12] By invoking the quantum de Finetti theorem one can prove that in the limit of large coordination number all possible ground states will be separable,[9,13] which in turn implies that mean-field theory becomes exact in the limit of infinite-dimensional lattices.

Due to the variational nature of ground states, there always exists a ground state with the same symmetries as the associated Hamiltonian. If the Hamiltonian has translational symmetry and consists of two-body nearest-neighbor interactions, then it is clear that the energy of a state with the right symmetry is completely determined by its reduced density operator of two neighboring spins. The reduced density operators arising from these (eventually mixed) states with a given symmetry form a convex set, and the energy for a given Hamiltonian will be minimized for a state whose reduced density operator is an extreme point in this set. More specifically, the equation $\mathrm{Tr}(H\rho) = E$ determines a hyperplane in the space of reduced density operators of states with a given symmetry, and the energy will be extremal when the hyperplane is tangent to the convex set ($E = E_{\mathrm{extr}}$). The problem of finding the ground state energy of nearest-neighbor translational invariant Hamiltonians is therefore equivalent to the determination of the convex set of two-body reduced density operators arising from states with the right symmetry. Strictly speaking, these two problems are dual to each other. In the case of quadratic Hamiltonians involving continuous
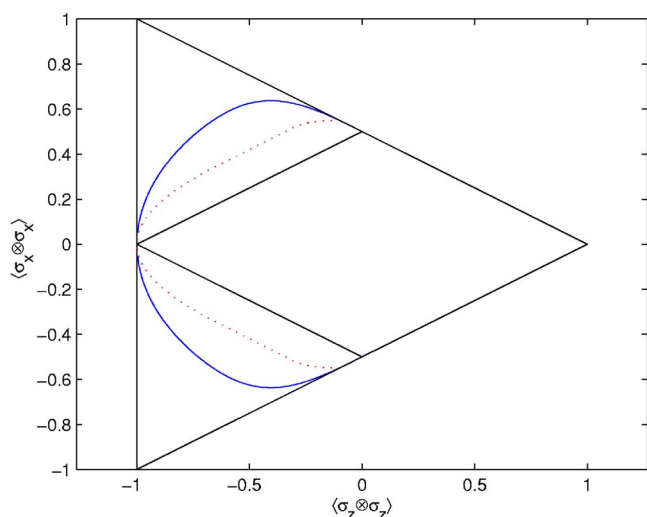
FIG. 1. (Color online) Convex sets of the possible reduced density operators of translational invariant states in the *XX-ZZ* plane: the big triangle represents all positive density operators, the inner parallellogram represents the separable states, the union of the separable cone and the convex hull of the full curved line is the complete convex set in the case of a 1D geometry, and the dashed lines represent extreme points in the 2D case of a square lattice. The singlet corresponds to the point with coordinates $(-1,-1)$.

variables, the determination of this convex set was solved for fairly general settings in Ref. 14 by means of Gaussian states. The determination of this convex set in the case of spin systems, however, turns out to be much more challenging.

Let us illustrate this with a simple example. Consider the *XXZ*-Hamiltonian with nearest-neighbor interactions

$$\mathcal{H} = -\sum_{\langle i,j\rangle} S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z$$

on a lattice of arbitrary geometry and dimension.[15] Due to the symmetries, the reduced density operator of two nearest neighbors can be parametrized by only two parameters[16]

$$\rho = \frac{1}{4}[\mathbb{1} \otimes \mathbb{1} + x(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y) + z\sigma_z \otimes \sigma_z].$$

Positivity of ρ enforces $-1 \leqslant z \leqslant 1-2|x|$, and the state is separable iff $1+z \leqslant 2|x|$. In the case of an infinite 1D spin chain, the ground-state energy $E(\Delta)$ has been calculated exactly,[17] and this determines the tangent hyperplanes

$$2x + z\Delta + E(\Delta) = 0$$

whose envelope makes up the extreme points of the convex set of reduced density operators of translationally invariant 1D states: the boundary of this convex set is parametrized by

$$z = -\partial E(\Delta)/\partial\Delta,$$

$$x = -[E(\Delta) + \partial E(\Delta)/\partial\Delta]/2,$$

which we plotted in Fig. 1. We also plot the boundary for the two-dimensional square lattice. These 2D data were obtained by numerical methods[18–20]; of course this convex set is con-

tained in the previous one, as all the semidefinite constraints defining the set corresponding to 1D are strictly included in the set of constraints for the 2D case. Finally, we plot the set of separable states, which contains the reduced density operators of the allowed states for a lattice with infinite coordination number. The boundary of this separable set is given by the inner diamond; this immediately implies that the difference between the exact energy and the one obtained by mean-field theory will be maximized whenever the hyperplane that forms the boundary of the first set will be parallel to this line. This happens when $\Delta = -1$ (independent of the dimension), which corresponds to the antiferromagnetic case, and this proves that the "entanglement gap"[12] in the *XXZ* plane is maximized by the antiferromagnetic ground state for any dimension and geometry. Similarly, it proves that the ground state is separable whenever $\Delta \geqslant 1$ and $\Delta = -\infty$. Note also that in the 2D case, part of the boundary of the convex set consists of a plane parametrized by $2x + z + E(1) = 0$. This indicates a degeneracy of the ground state around the antiferromagnetic point, and indicates that a phase transition is occurring at that point (more specifically between an Ising and a Berezinskii-Kosterlitz-Thouless phase). It would be very interesting to investigate this further, and it is fascinating that this phase transition could be detected by just looking at the structure of these low-dimensional convex sets.

The previous discussion implies that ground states of quantum spin systems are very special: they are completely determined by their two-body reduced density operators. Typically, it even holds that the ground state of an interacting spin system is unique, which implies that most extreme points in the convex set of reduced density operators uniquely characterize a state with the right symmetry properties. This is very good news if we want to create families of variational ground states: it suffices to approximate well the local properties of all translational invariant states. The family of matrix product states (MPSs)[3,21,22] and generalizations to higher dimensions (PEPS)[18,23,24] were exactly created with this property in mind; the amazing accuracy of renormalization group algorithms is precisely related to the fact that the convex set under consideration can be very well approximated with the reduced density operators of MPS. Both Wilson's numerical renormalization group[1] and density matrix renormalization group (DMRG)[2,25] methods can indeed be reformulated as variational methods within the MPS.[4,22]

The reason why ground states of gapped quantum spin systems can be parametrized as MPS/PEPS can be understood by the following handwaving argument. A celebrated theorem of Hastings[26] states that in the case of a gapped system all correlations are decaying exponentially. Let us therefore consider a 1D gapped quantum spin system with correlation length ξ_{corr}. Due to the finite correlation length, the reduced density operator ρ_{AB} obtained when tracing out a block C of length $l_{AB} \gg \xi_{corr}$ (see Fig. 2) is expected to be of the form[27]

$$\rho_{AB} \simeq \rho_A \otimes \rho_B$$

up to exponentially small corrections. Clearly, the original ground state $|\psi_{ABC}\rangle$ is a purification of this mixed state, but it
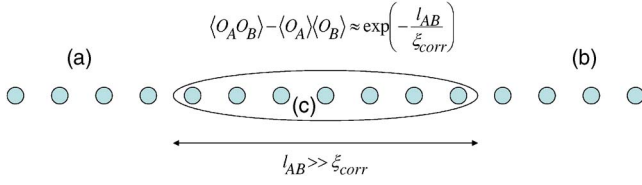
FIG. 2. (Color online) A one-dimensional spin chain with finite correlation length ξ_{corr}; l_{AB} denotes the distance between the block A (left) and B (right). Because l_{AB} is much larger than the correlation length ξ_{corr}, the state ρ_{AB} is essentially a product state.

is of course also possible to find a purification of the form $|\psi_{AC_l}\rangle \otimes |\psi_{BC_r}\rangle$ (up to exponentially small corrections) with no correlations whatsoever between A and B; here C_l and C_r together span the original block C. It is, however, well known that all possible purifications of a mixed state are equivalent to each other up to local unitaries on the ancillary Hilbert space. This automatically implies that there exists a unitary operation U_C on the block C (see Fig. 2) that completely disentangles the left from the right part:

$$\mathbb{1}_A \otimes U_C \otimes \mathbb{1}_B |\psi_{ABC}\rangle \simeq |\psi_{AC_l}\rangle \otimes |\psi_{BC_r}\rangle.$$

This implies that there exists a tensor $A^i_{\alpha,\beta}$ with indices $1 \leq \alpha, \beta, i \leq D$ (where D is the dimension of the Hilbert space of C) and states $|\psi^A_\alpha\rangle, |\psi^C_i\rangle, |\psi^B_\beta\rangle$ defined on the Hilbert spaces belonging to A, B, C such that

$$|\psi_{ABC}\rangle \simeq \sum_{\alpha,\beta,i} A^i_{\alpha,\beta} |\psi^A_\alpha\rangle |\psi^C_i\rangle |\psi^B_\beta\rangle.$$

Applying this argument recursively leads to a MPS [to be defined in Eq. (1)] and indeed hints that ground states of gapped Hamiltonians are well represented by MPS. In this paper we will show that this even holds for critical systems.

As a good illustration of the actual accuracy obtained with MPS, we calculated the convex set obtained with MPS in the thermodynamic limit for the XXZ-chain with $D=2$, where D is the dimension of the matrices in the MPS (see Fig. 3). It is almost unbelievable how good the exact convex set can be approximated. Note that typical DMRG calculations have $D \sim 200$, and that the accuracy grows superpolynomial in D. Note also that the $D=1$ case corresponds to mean-field theory, whose corresponding convex set coincides with the set of separable states.

The same argument involving the notion of a correlation length applies in higher dimensions and indicates that PEPS represent ground states of gapped local Hamiltonians well. Note however that the convex set in the 2D case is much closer to the separable one than in the 1D case; this gives a hint that PEPS of smaller dimension will suffice to give the same accuracy as in the 1D case. In the next section we will quantitatively bound how well a translationally invariant state can be represented in terms of a MPS, and will analyze the corresponding implications for the description of ground states of 1D spin chains.
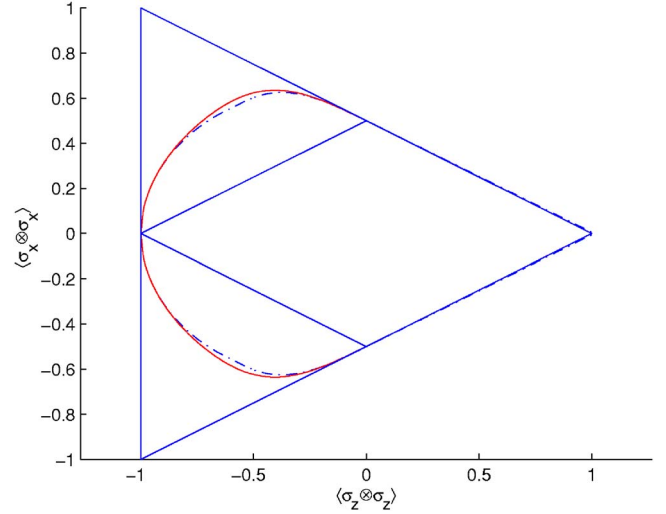

FIG. 3. (Color online) Convex sets in the XXZ plane: the inner diamond borders the set of separable states (see Fig. 1). Dash-dotted: extreme points of the convex set produced by MPS of $D=2$.

III. ANALYTICAL BOUNDS FOR MATRIX PRODUCT STATES

Let us start by recalling the expression of D-dimensional MPS describing N spins of dimension d,

$$|\psi_D\rangle = \sum_{i_1,\dots,i_N=1}^d \text{tr}[A^{[1]i_1}\dots A^{[N]i_N}]|i_1,\dots,i_N\rangle. \quad (1)$$

Here, $A^{[k],1},\dots,A^{[k],d}$ are, in general, $D_k \times \widetilde{D}_k$ complex matrices, with $D_{k+1}=\widetilde{D}_k \leq D$.

We will show first how well one can describe general states in terms of MPS. We will choose $D_1=\widetilde{D}_N=1$, i.e., $A^{[1]i_1}$ and $A^{[N]i_N}$ will be vectors. In this case, one can impose the following *gauge* condition:[28,29]

$$\sum_i A^{[m]i}A^{[m]i\dagger} = \mathbb{1}, \quad \sum_i A^{[m]i\dagger}\Lambda^{[m+1]}A^{[m]i} = \Lambda^{[m]}. \quad (2)$$

Here $\Lambda^{[m]}$ represents the diagonal matrix with the corresponding eigenvalues $\{\widetilde{\lambda}^{[m]i}\}$ sorted in decreasing order, i.e., $\widetilde{\lambda}^{[m]1} \geq \widetilde{\lambda}^{[m]2} \geq \cdots$. We consider an arbitrary state $|\psi\rangle$ and denote by

$$\{\mu^{[\alpha]i}\}, \quad i=1\cdots N_\alpha = d^{\min(\alpha,N-\alpha)}$$

the eigenvalues of the reduced density operators

$$\rho_\alpha = \text{Tr}_{\alpha+1,\alpha+2,\dots,N}|\psi\rangle\langle\psi|,$$

also sorted in decreasing order. In the following we will investigate (i) how well a general quantum state can be approximated by a D-dimensional MPS and (ii) how well the reduced density operators of a translationally invariant state can be described by the one corresponding to a D-dimensional MPS.

A. General states: Analytic results and implications

We start out with the main result of this paper, which gives an upper bound to the error made by approximating a general state by a MPS. As we will show below, this has very important implications in the performance of the renormalization algorithms to describe ground states of 1D spin chains.

Lemma 1. There exists a MPS $|\psi_D\rangle$ of dimension D such that

$$\||\psi\rangle - |\psi_D\rangle\|^2 \leq 2\sum_{\alpha=1}^{N-1} \epsilon_\alpha(D),$$

where $\epsilon_\alpha(D) = \Sigma_{i=D+1}^{N_\alpha}\mu^{[\alpha]i}$.

Proof. We can always write ψ as a MPS of dimension $D = 2^{N/2}$ and fulfilling Eq. (2). Let us now consider the D-dimensional MPS $|\psi_D\rangle$ which is defined by the $D \times D$ matrices $[A^{[\alpha]i}]_{(1\ldots D,1\ldots D)}$ (i.e., the upper-left block of $A^{[\alpha]i}$). The goal is now to bound $\langle\psi|\psi_D\rangle$. The gauge conditions were chosen such as to make the task simple

$$\langle\psi_D|\psi\rangle = \mathrm{Tr}(\$_2\{\cdots\$_{N-2}[\$_{N-1}(\Lambda^{N-1}P)P]P\cdots\}P); \quad (3)$$

here $P = \Sigma_{k=1}^D|k\rangle\langle k|$ and $\$_m(X) = \Sigma_i A^{[m]i\dagger}XA^{[m]i}$ represents a trace-preserving completely positive (TPCP) map parametrized by the Kraus operators $A^{[m]i}$. Let us now recursively define

$$Y^{[k]} = \$_k(Y^{[k+1]}P), \quad Y^{[N-1]} = \Lambda^{[N-1]}P;$$

observe that $\Lambda^{[k]} = \$_k(\Lambda^{[k+1]})$. We want a bound on $\mathrm{Tr}|\Lambda^{[1]} - Y_1|$, as Eq. (3) is equal to $\mathrm{Tr}(Y^{[2]})$. The crucial property we need is that TPCP maps are contractive with relation to the trace-norm[30] $\mathrm{Tr}|\$(X)| \leq \mathrm{Tr}|X|$. It follows that

$$\mathrm{Tr}|\Lambda^{[k]} - Y^{[k]}| = \mathrm{Tr}|\$_k(\Lambda^{[k+1]} - Y^{[k+1]}P)|$$

$$\leq \mathrm{Tr}|\Lambda^{[k+1]} - Y^{[k+1]}P|$$

$$\leq \mathrm{Tr}|\Lambda^{[k+1]} - Y^{[k+1]}| + \mathrm{Tr}|\Lambda^{[k+1]}(1 - P)|.$$

Note that the last term in the sum is exactly given by $\Sigma_{\alpha=D+1}^{2^{N/2}}\lambda^{[k+1]\alpha}$. The theorem now follows immediately by recursion and by observing that $\langle\psi_D|\psi_D\rangle \leq 1$ by similar arguments. ∎

The implications of this result are very strong: it shows that for systems for which the $\epsilon_\alpha(D)$ decay fast in D, there exist MPS with *small D* which will not only reproduce well the local correlations (such as energy) but also all the nonlocal properties (such as correlation length). The following lemma now relates the derived bound to the Renyi entropies of the reduced density operators, through which one can make the connection to the ground states of 1D Hamiltonians. The Renyi entropies of ρ are defined as

$$S^\alpha(\rho) = \frac{1}{1-\alpha}\ln(\mathrm{Tr}\,\rho^\alpha),$$

and we will consider $0 < \alpha < 1$. We denote as before $\epsilon(D) = \Sigma_{i=D+1}^\infty\lambda_i$ with λ_i the nonincreasingly ordered eigenvalues of ρ. Then we have the following.

Lemma 2. Given a density operator ρ, if $0 < \alpha < 1$, then $\ln[\epsilon(D)] \leq (1-\alpha)/\alpha[S^\alpha(\rho) - \ln(D/(1-\alpha))]$.

Proof. Let us first characterize the probability distribution that has maximal possible weight in its tail (i.e., $p = \Sigma_{i=D+1}^\infty p_i$) for a given Renyi entropy. Introducing a free parameter $0 < h \leq (1-p)/D$, such a probability distribution must be of the form

$$p_1 = 1 - p - (D-1)h,$$

$$h = p_2 = p_3 = \cdots p_{D+p/h},$$

$$p_{D+p/h+1}, \ldots, p_\infty = 0$$

because this distribution majorizes all other ones with given p, D, p_D (Renyi entropies are Schur-convex functions). For a given p, D, h, it holds that

$$\sum_i p_i^\alpha = [1 - p - (D-1)h]^\alpha + (D - 1 + p/h)h^\alpha$$

$$\geq Dh^\alpha + ph^{\alpha-1}.$$

Minimizing this expression with relation to h, we get

$$\sum_i p_i^\alpha \geq (D^{1-\alpha}p^\alpha)/[(1-\alpha)^{1-\alpha}\alpha^\alpha].$$

Denoting $S^\alpha(p,D)$ the minimal possible entropy for given p, D, we get

$$S^\alpha(p,D) \geq \frac{1}{1-\alpha}\ln\left(\frac{D^{1-\alpha}p^\alpha}{(1-\alpha)^{1-\alpha}\alpha^\alpha}\right)$$

and hence

$$p \leq \exp\left[\frac{1-\alpha}{\alpha}\left(S^\alpha(p,D) - \log\frac{D}{1-\alpha}\right)\right].$$

The proof now follows by replacing $S^\alpha(p,D)$ by $S^\alpha(\rho)$. ∎

This lemma is very interesting in the light of the fact that in the case of critical systems, arguable the hardest ones to simulate,[31] the Renyi-entropy of a contiguous block of L spins scales as[32–36]

$$S^\alpha(\rho_L) \simeq \frac{c + \bar{c}}{12}\left(1 + \frac{1}{\alpha}\right)\ln(L) \quad (4)$$

for all $\alpha > 0$; here c is the central charge. The fact that the eigenvalues of ρ_L decay fast has previously been identified as a indication for the validity of the DMRG approach.[32] The truncation error,[2,25] which has been used in the DMRG community as a check for convergence, is essentially given by $\epsilon(D) - \epsilon(2D)$ and therefore indeed gives a good idea of the error in a simulation.

Let us investigate how the computational effort to simulate such critical systems scales as a function of the length $N = 2L$ of the chain. Let us therefore consider the Hamiltonian associated to a critical system, but restrict it to $2L$ sites. The entropy of a half chain (we consider the ground state $|\psi_{ex}\rangle$ of the finite system) will typically scale as in Eq. (4) but with an extra term that scales as $1/N$. Suppose we want to enforce that $\||\psi_{ex}\rangle - |\psi_D\rangle\|^2 \leq \epsilon_0/L$ with ϵ_0 indepen-

dent of L.[37] Denote the minimal D needed to get this precision for a chain of length $2L$ by D_L. Following lemma (1) and the fact that the entropy of all possible contiguous blocks reaches its maximum in the middle of the chain (hence $p \leqslant \epsilon_0/L^2$ is certainly sufficient), lemmas (1) and (2) combined yield

$$D_L \leqslant cst\left(\frac{L^2}{(1-\alpha)\epsilon_0}\right)^{\alpha/(1-\alpha)} L^{(c+\bar{c})/12(1+\alpha)\alpha}.$$

This shows that D only has to scale polynomially in L to keep the accuracy ϵ_0/L fixed; in other words, there exists an efficient scalable representation for ground states of critical systems (and hence also of noncritical systems) in terms of MPS! Such a strong result could not have been anticipated from just doing simulations.

Now what about the complexity of finding this optimal MPS? It has been observed that DMRG converges exponentially fast to the ground state with a relaxation time proportional to the inverse of the gap Δ of the system.[25] For translational invariant critical systems, this gap seems to close only polynomially. As we have proven that D only have to scale polynomially too, the computational effort for finding ground states of 1D quantum systems is polynomial (P). Let us recapitulate for which systems and under which conditions this statement is true: (1) the α entropy of blocks in the exact ground state grow at most logarithmically with the size of the block for some $\alpha < 1$, (2) the gap of the system scales at most polynomially with the system size, (3) given a gap that obeys condition 2, there exists an efficient DMRG-like algorithm that converges to the global minimum. As the variational MPS approach[22] is essentially an alternating least squares method of solving a nonconvex problem, there is a priori no guarantee that it will converge to the global optimum,[38] although the occurrence of local minima seems to be very unlikely.[25] Note that this, e.g., implies that there would be no exponential gain in using a quantum computer in simulating 1D spin systems, as the steps needed in a quantum computer are also bounded by the inverse of the gap.

B. Reduced density operators of translationally invariant states

Now we turn to the study of how MPS approximate the local properties of translationally invariant states ψ of $N \rightarrow \infty$ systems. Let us denote by ψ a translationally invariant state with $N = \infty$ and by $\sigma = \text{tr}(\rho)$ the corresponding two-particle reduced density operator, where the trace is taken with respect to all particles except for two neighbors (say particles 1 and 2). Our goal is to show that there exists a D-dimensional MPS whose corresponding reduced density operator σ_D approximates well σ. More specifically, we want to bound $\|\sigma - \sigma_D\|_1$ from above. Note that any nearest neighbor correlation function, and in particular the energy density will be automatically bounded.

One can represent the state[39] ψ as a MPS (1) with all the A's equal and $D, N = \infty$. Without loss of generality we can again choose the *gauge* condition (2) with A, Λ site independent. In fact, the elements Λ_{ii} coincide with the eigenvalues λ_i of the reduced density operator corresponding to half a chain. As before, they will play a very important role in the bound that we derive; in particular, we will need $\epsilon(D) = \Sigma_{\alpha=D+1}^{\infty} \lambda_\alpha$ and we define

$$\gamma_D = \left(\sum_{\alpha=1}^{D} \sqrt{\lambda_\alpha}\right)\sum_{\beta=1}^{D}\sum_{n=1}^{\infty} \frac{\lambda_{\beta+Dn}}{\sqrt{\lambda_\beta}}$$

which roughly behaves as $\epsilon(D)$, i.e., it becomes small when D is large.

Lemma 3. Given ψ and σ as defined above, there exists a D-dimensional MPS such that

$$\frac{1}{d^2}\,\text{Tr}|\sigma - \sigma_D| \leqslant 2[\sqrt{\epsilon(D)} + \epsilon(D)] + \gamma_D. \qquad (5)$$

Proof. One can easily show that

$$r^{i,i',j,j'} \equiv \langle i|\langle i'|\rho|j\rangle|j'\rangle = \text{Tr}[A^{j\dagger}\Lambda A^i A^{i'} A^{j'\dagger}]$$

$$= \sum_{\alpha,\beta,n,m} [A^{j\dagger}\Lambda A^i]_{\alpha+Dn,\beta+Dm}[A^{i'} A^{j'\dagger}]_{\beta+Dm,\alpha+Dn}.$$

Let us consider the D-dimensional matrix product density operator[40] (MPDO)

$$\rho_D = \sum \text{Tr}(B^{i_1 j_1} \cdots B^{i_\infty j_\infty})|i_1\rangle \cdots |i_\infty\rangle\langle j_1| \cdots \langle j_\infty|$$

parametrized by

$$B^{ij}_{\alpha\alpha';\beta\beta'} = \sum_{n,m} A^i_{\alpha+Dn,\beta+Dm}A^{*j}_{\alpha'+Dn,\beta'+Dm}x_{\alpha,n}x_{\alpha',n},$$

$$x_{\alpha,n} = \sqrt{\frac{\lambda_{\alpha+Dn}}{\sum_{m=0}^{\infty} \lambda_{\alpha+Dm}}}.$$

The following eigenvalue equations are easily verified:

$$\sum B^{ii}_{\alpha\alpha';\beta\beta'}\delta_{\alpha'\beta'} = \delta_{\alpha\beta},$$

$$\sum B^{ii}_{\alpha\alpha';\beta\beta'}\tilde{\Lambda}_{\alpha\beta} = \tilde{\Lambda}_{\alpha'\beta'},$$

where

$$\tilde{\Lambda}_{\alpha\beta} = \delta_{\alpha\beta}\sum_{k=0}^{\infty} \lambda_{\alpha+Dk}.$$

The reduced density operator $s^{i,i',j,j'} \equiv \langle i|\langle i'|\rho_D|j\rangle|j'\rangle$ is given by

$$\sum_{\alpha\beta nm} [A^{j\dagger}\Lambda A^i]_{\alpha+Dn,\beta+Dn}[A^{i'} A^{j'\dagger}]_{\beta+Dm,\alpha+Dm}x_{\beta,m}x_{\alpha,m}. \quad (6)$$

We divide r and s in two parts

$$r^{i,i',j,j'} = r_0^{i,i',j,j'} + r_1^{i,i',j,j'},$$

$$s^{i,i',j,j'} = s_0^{i,i',j,j'} + s_1^{i,i',j,j'}.$$

The first parts (r_0 and s_0) contain just the part of the sums with $n = m = 0$, whereas the second ones (r_1 and s_1) contain the rest of the sums.

The goal is to find upper bounds for

$$\Delta r = \sum_{i,i',j,j'=1}^{d} |r_1^{i,i',j,j'}|,$$

$$\Delta s = \sum_{i,i',j,j'=1}^{d} |s_1^{i,i',j,j'}|,$$

$$\Delta t = \sum_{i,i',j,j'=1}^{d} |r_0^{i,i',j,j'} - s_0^{i,i',j,j'}|.$$

We start with Δr. We can write

$$\Delta r = \sum_{i,i',j,j'=1}^{d} |\text{Tr}[A^{j\dagger}\Lambda A^i P A^{i'} A^{j'\dagger}] + \text{Tr}[P A^{j\dagger}\Lambda A^i A^{i'} A^{j'\dagger}]|. \tag{7}$$

Here,

$$P = \sum_{x=D}^{\infty} |x\rangle\langle x|$$

with $|x\rangle$ a unit vector in the computational basis. Using Cauchy-Schwartz inequality we have

$$\sum_{i,i',j,j'=1}^{d} |\text{Tr}[A^{j\dagger}\Lambda A^i P A^{i'} A^{j'\dagger}]|$$

$$\leq \left[\sum_{i,i',j,j'=1}^{d} \text{Tr}[A^{i'\dagger} P A^{i\dagger}\Lambda A^i P A^{i'}] \right]^{1/2}$$

$$\times \left[\sum_{i,i',j,j'=1}^{d} \text{Tr}[A^{j'\dagger} A^{j\dagger}\Lambda A^j A^{j'}] \right]^{1/2}$$

$$= d^2 (\text{Tr}[P\Lambda P])^{1/2} = d^2 \sqrt{\sum_{x=D}^{\infty} \lambda_x}.$$

The second term in Eq. (7) gives the same, so that we have

$$\Delta r \leq 2d^2 \sqrt{\sum_{x=D}^{\infty} \lambda_x} = 2d^2 \sqrt{\epsilon(D)}.$$

The term Δs is a bit more tricky. We write it as

$$\Delta s = \sum_{n,m}{}' \sum_{x,y} \sum_{i,i',j,j'=1}^{d} L_{x,y,n,m}^{ii'} L_{x,y,n,m}^{jj'*},$$

where the prime in the sum means that $n=m=0$ is excluded, and

$$L_{x,y,n,m}^{ii'} = \sqrt{\lambda_x} \sum_{\beta} x_{\beta,m} A_{x,\beta+Dn}^{i} A_{\beta+Dm,y}^{i'}.$$

Using Cauchy-Schwartz inequality we get

$$\Delta s \leq \sum_{n,m}{}' \sum_{x,y} \sum_{i,i',j,j'=1}^{d} |L_{x,y,n,m}^{ii'}|^2$$

$$= d^2 \sum_{n,m}{}' \sum_{\beta} \frac{\lambda_{\beta+Dn}\lambda_{\beta+Dm}}{\sum_k \lambda_{\beta+Dk}} \leq 2d^2 \sum_{\beta} \sum_{n=1}^{\infty} \lambda_{\beta+Dn}$$

$$\leq 2d^2 \sum_{x=D}^{\infty} \lambda_x = 2d^2 \epsilon(D).$$

Now, it only remains to bound Δt. Again making use of the Cauchy-Schwartz inequality and the inequality

$$\left| 1 - \frac{1}{1+x}\frac{1}{1+y} \right| \leq x + y$$

we get

$$\Delta t \leq d^2 \sum_{\alpha=1}^{D} \sqrt{\lambda_\alpha} \sum_{\beta=1}^{D} \sum_{n=1}^{\infty} \frac{\lambda_{\beta+Dn}}{\sqrt{\lambda_\beta}}.$$

The bound states in the lemma is given by $\Delta r + \Delta s + \Delta t$. ∎

The usefulness of this lemma relies in the fact that the spectrum $\{\lambda^i\}$ is typically decaying very fast for noncritical systems, and hence the upper bound decays typically very fast with increasing D. Let us illustrate this on the hand of, e.g., the *XXZ* Hamiltonian on a chain

$$\mathcal{H} = -\sum_{\langle i,j\rangle} S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z.$$

For $\Delta < -1$, the spectrum of the halve-infinite chain can be calculated exactly.[32] All eigenvalues are of the form $c(z)z^n$ where

$$z = \exp[-2\,\text{arcosh}(|\Delta|)],$$

$$1/c(z) = \sum_{n=0}^{\infty} a(n)z^n,$$

and where $a(n)$ denotes the degeneracy of each eigenvalue and is given by the number of possible partitions of n into odd parts. The asymptotics of $a(n)$ are known exactly:[41]

$$a(n) \sim \frac{1}{4} \frac{e^{(\pi/\sqrt{3})\sqrt{n}}}{3^{1/4}n^{3/4}}.$$

To determine the power $n(D)$ of the $(D+1)$th largest eigenvalue $c(z)z^n(D)$ (taking into account degeneracy off course), we have solve the equation

$$D = \sum_{m=0}^{n(D)} a(m)$$

for $n(D)$. Asymptotically, this becomes

$$D \sim \frac{3^{1/4}}{2\pi} \frac{e^{(\pi/\sqrt{3})\sqrt{n(D)}}}{n(D)^{1/4}}, \quad n(D) \sim \left(\frac{\ln(D)}{\pi/\sqrt{3}}\right)^2.$$

$\epsilon(D)$, the sum of all eigenvalues smaller than the D largest ones, can now readily be calculated as

$$\epsilon(D) = c(z) \sum_{m=n(D)}^{\infty} a(m) z^m \sim \exp\left(-\frac{3|\ln z|}{\pi^2} (\ln D)^2 \right).$$

This last expression decays faster than any inverse power of D. A similar calculation holds for γ_D, showing that the upper bound in lemma 3 decays faster than any polynomial in D. This is a very nice illustration for the superpolynomial accuracy of the infinite DMRG method for the *XXZ* model. The other integrable models will have a very similar behavior, and it is expected that non-integrable models share the same features. Of course, the upper bounds derived here are not tight, and in practice the accuracy of a DMRG will be much better than derived here.

IV. CONCLUSION

In conclusion, we highlighted the importance of the concept of local reduced density operators of translational invariant systems, their approximation using matrix product states, and the connection with frustration and monogamy properties of entanglement. We quantified how well matrix product states approximate exact ground states of 1D quantum spin systems as a function of the entropy of blocks of spins, and showed that the complexity for representing ground states of 1D systems (even critical ones) as MPS scales polynomially in the number of spins.

ACKNOWLEDGMENTS

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