Infinite matrix product states, conformal field theory, and the Haldane-Shastry model

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(Received 26 November 2009; revised manuscript received 19 February 2010; published 31 March 2010)

We generalize the matrix product states method using the chiral vertex operators of conformal field theory and apply it to study the ground states of the XXZ spin chain, the J_1-J_2 model and random Heisenberg models. We compute the overlap with the exact wave functions, spin-spin correlators, and the Renyi entropy, showing that critical systems can be described by this method. For rotational invariant ansatzs we construct an inhomogenous extension of the Haldane-Shastry model with long-range exchange interactions.

DOI: 10.1103/PhysRevB.81.104431 PACS number(s): 05.10.Cc, 03.67.Bg, 03.67.Mn, 11.25.Hf

In recent years the study of one-dimensional (1D) quantum lattice systems has received an enormous impetus due to the invention of numerical algorithms, such as the density matrix renormalization group (DMRG) (Ref. 1) and its extensions (for a review see Ref. 2). The key for the success of those methods is the careful treatment of the complex structure of the low-energy states, which is based on the behavior of the entanglement entropy at zero temperature.[3] For a gapped system, the entanglement entropy, S_L, of a subsystem of length L converges toward a constant value, independent of L.[4] For critical systems, however, S_L grows as the logarithm of L, were the proportionality factor is related to the central charge c of the underlying conformal field theory (CFT).[5] This behavior of S_L implies[6] that the ground state (GS) of the system is well approximated by a matrix product state (MPS),[7] a state characterized in terms of certain matrices A_s. This explains the enormous success of DMRG since it can be understood as a variational method with respect to MPS of bounded dimension.[8] However, the unbounded increase in the entanglement entropy makes DMRG much less accurate for critical systems since the size of the matrices characterizing the MPS must inevitably grow with the size of the system. Thus, in order to properly describe the low-energy states of such systems MPS with infinitely dimensional matrices A_s are required.

The purpose of this paper is to construct such infinite-dimensional MPS (iMPS for short) and their application to 1D spin chains. We will replace the finite-dimensional matrices A_s by chiral vertex operators of a CFT. These operators act on infinite-dimensional Hilbert spaces, which acquire the meaning of ancillary space where entanglement and correlations are transported. The huge enlargement of the ancillary space will allow us to describe both critical and noncritical 1D systems on equal footing. In particular, we will consider the XXZ and J_1-J_2 models to illustrate the accuracy of our method.

Whereas standard MPS have, in general, a complicated form if written in the spin basis, the iMPS that we shall consider below have a rather simple form given by Jastrow-type wave functions. There exists many important examples of that type of wave functions, such as the Laughlin state of the fractional quantum Hall effect (FQHE),[9] the Haldane-Shastry state (HS) of the inverse square Heisenberg model[10] and the related Calogero-Sutherland state of hard-core bosons.[11] A particular example of iMPS, which has spin rotational invariance, will coincide with the HS wave function. This case is particularly interesting because there is an enhanced symmetry described by the $SU(2)_k$ Wess-Zumino-Witten (WZW) model at level $k=1$. Using the Ward identities of this CFT we shall find an integrable extension of the HS Hamiltonian parameterized by a large number of coefficients. We will then use this extended HS model to study the entanglement entropy of spin chains with frustration and random couplings, finding a very good agreement with a law recently proposed in Refs. 20 and 21.

Let us consider a spin-1/2 chain with N sites, and local spin basis $|s_i\rangle$, where $s_i=\pm 1$ $(i=1,\ldots,N)$. A generic state in the Hilbert space of this spin chain is given by

$$|\psi\rangle = \sum_{s_1,\ldots,s_N} \psi(s_1,\ldots,s_N)|s_1,\ldots,s_N\rangle. \quad (1)$$

A MPS state is an ansatz of the form

$$\psi(s_1,\ldots,s_N) = \langle u|A^{(1)}_{s_1}\cdots A^{(N)}_{s_N}|v\rangle, \quad (2)$$

where $A^{(i)}_{s_i}$ and $\langle u|,|v\rangle$ are D-dimensional matrices and row and column vectors, respectively. The number or parameters needed to specify a MPS scales as $2D^2N$, which is much smaller than the number of components of a generic state, Eq. (1), namely, 2^N. To define a iMPS we shall replace the matrices $A^{(i)}_{s_i}$ by the chiral vertex operators of a CFT, thus effectively working with $D=\infty$. Let us choose for simplicity a Gaussian CFT with central charge $c=1$. Chiral vertex operators are normal-ordered exponentials of the chiral bosonic field $\varphi(z)$,[12] which we can be used to define

$$A^{(i)}_{s_i} = \chi_{s_i} :e^{i s_i \sqrt{\alpha}\varphi(z_i)}: \quad (i=1,\ldots,N), \quad (3)$$

where z_i are complex numbers, α a positive real number, $\chi_{s_j}=1$ for j even, and $\chi_{s_j}=e^{i\pi(s_j-1)/2}$ for j odd.[13] The scaling dimension of these operators is $h=\alpha/2$. For the vectors $\langle u|,|v\rangle$, we take the outgoing and incoming vacuum states of the Gaussian CFT. Equation (2) becomes then the vacuum expectation value of a product of vertex operators which is given by[12]

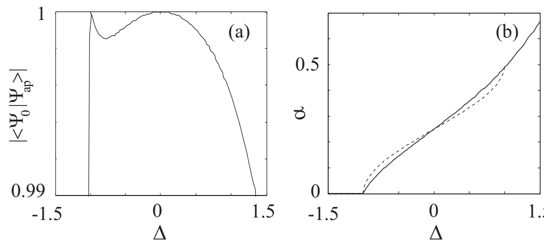

FIG. 1. (a) Overlap of the variational ansatz, Eq. (5), with the exact GS wave function of Hamiltonian (7) in the sector with $S^z=0$ for $N=20$ spins; (b) optimal value of α. The dashed line shows the curve $\Delta=-\cos(2\pi\alpha)$.

$$\psi(s_1,\ldots,s_N)=\delta_s e^{i\pi/2\sum_{i:\mathrm{odd}}(s_i-1)}\prod_{i>j}^{N}(z_i-z_j)^{\alpha s_i s_j}, \qquad (4)$$

where $\delta_s=1$ if $\sum_{i=1}^N s_i=0$ and zero otherwise. This condition can be traced back to the conservation of the $U(1)$ charge of the Gaussian CFT. Equation (3) associates the charge of the vertex operator $A_{s_i}^{(i)}$ to the local spin s_i, so that the total third component of the spin, $S^z=\sum_i s_i/2$, vanishes. We will use the iMPS variationally with z_i and α as variational parameters. The wave function (4) scales with an overall factor under a Moebius transformation $z_i\to(az_i+b)/(cz_i+d)\ \forall i$, so that the ansatz only depends on $N-3$ z parameters. The latter parameters must not be identified with the position of the local spins s_i. An exception is the wave function associated to translationally invariant spin chains where we shall choose $z_n=e^{2\pi i n/N}(n=1,\ldots,N)$. In that case we have

$$\psi(s_1,\ldots,s_N)\propto\delta_s e^{i\pi/2\sum_{i:\mathrm{odd}}s_i}\prod_{n>m}^{N}\left[\sin\frac{\pi(n-m)}{N}\right]^{\alpha s_n s_m}. \qquad (5)$$

For later purposes, it is convenient to express this spin wave function using hard-core boson variables. Let $q_i=0,1$ be the occupation number of a hard-core boson at the site i. Mapping the spin-up (down) states into empty (occupied) hard-core boson states, amounts to the relation $s_i=1-2q_i$. The wave function (5) then becomes

$$\psi(n_1,\ldots,n_{N/2})\propto e^{i\pi\sum_i n_i}\prod_{n_i>n_j}^{N/2}\left[\sin\frac{\pi(n_i-n_j)}{N}\right]^{4\alpha}, \qquad (6)$$

where $n_i=1,\ldots,N$ denote the positions of $N/2$ hard-core bosons in the lattice (i.e., those points where $q_{n_i}=1$).

(1) *The XXZ spin chain.* The Hamiltonian with anisotropic coupling Δ is given by

$$H_{\mathrm{XXZ}}=\sum_{i=1}^{N}(S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+\Delta S_i^zS_{i+1}^z), \qquad (7)$$

where $\mathbf{S}_{N+1}=\mathbf{S}_1$ for periodic boundary conditions (we take N to be even). This model displays three different phases at zero temperature: (i) a gapped antiferromagnetic (AF) phase ($\Delta>1$), (ii) a critical phase ($-1<\Delta\leq 1$), and (iii) a ferromagnetic phase $\Delta\leq -1$. To describe the GS of the XXZ chain we shall use the translational invariant state, Eq. (5), which favors antiparallel nearest-neighbor spins. We expect this ansatz to adequately describe the $\Delta>-1$ regimes. The only variational parameter left in Eq. (5) is α, which we fix by numerically minimizing the energy. In Fig. 1 we plot this overlap as a function of Δ for $N=20$. As anticipated above, the overlap is rather poor in the ferromagnetic regime but surprisingly good for $\Delta>-1$, even above 99%. Moreover, the overlap is exactly one at $\Delta=0$ and -1, where $\alpha=1/4$ and 0, respectively. This indicates that the corresponding iMPS states coincide with the exact GS. To prove this result, one applies the unitary transformation $U=\Pi_{i:\mathrm{odd}}(2S_i^z)$ to Eq. (7) which flips the signs of the XY exchange interactions. For $\Delta=-1$, one obtains the isotropic ferromagnetic Heisenberg Hamiltonian, whose GS is fully polarized with $S^z=N/2$. Applying the lowering operator $(S^-)^{N/2}$ to this state, and undoing the unitary transformation, one recovers Eq. (5) for $\alpha=0$. For $\Delta<-1$ the rotational symmetry is broken and the unique GS is the fully polarized state with $S^z=N/2$, which is of course orthonormal to our $S^z=0$ ansatz. In the case $\Delta=0$, the transformed Hamiltonian describes free hard-core bosons, whose GS is the absolute value of a Slater determinant which yields

$$f(n_1,\ldots,n_{N/2})\propto\prod_{n_i>n_j}^{N/2}\sin\frac{\pi(n_i-n_j)}{N}, \qquad (8)$$

where $n_1,\ldots,n_{N/2}$ are the positions of the bosons on the lattice. Undoing the U transformation, one recovers the state, Eq. (6), with $\alpha=1/4$. For the isotropic XXX model, $\Delta=1$, the maximal overlap is obtained for $\alpha=1/2$. This value of α implies that the scaling dimension of the vertex operators $A_{s_i}^{(i)}$ is $h=1/4$, which coincides with that of the primary fields of spin 1/2 of the $\mathrm{SU}(2)_1$ WZW model. The corresponding wave function (5) does not yield the exact GS, but its hard-core version, Eq. (6), coincides with the GS of the Haldane-Shastry model, which belongs to the same universality class that the XXX chain (see below for a more detailed discussion).

Collecting the previous results we see that the iMPS ansatz, Eq. (5), in the range $0<\alpha\leq 1/2$, corresponds to the critical XXZ chain. To confirm the critical properties of this ansatz we have computed the Renyi entropy $S_L^{(2)}=-\log\mathrm{Tr}\,\rho_L^2$, where ρ_L is the density matrix of Eq. (5) restricted to a subsystem of size L. The computation is performed as follows. We rewrite

$$e^{-S_L^{(2)}}=\sum_{n,n',m,m'}|\langle n,m|\psi\rangle|^2|\langle n',m'|\psi\rangle|^2\frac{\langle\psi|n',m\rangle\langle\psi|n,m'\rangle}{\langle\psi|n,m\rangle\langle\psi|n',m'\rangle}, \qquad (9)$$

where $|n\rangle$ (and $|n'\rangle$) is an orthonormal basis in the space of the L spins and $|m\rangle$ (and $|m'\rangle$) another corresponding to the rest of spins. This expression can be easily evaluated by using two independent spin chains and performing the additions using Monte Carlo techniques. In Figs. 2(a)–2(c) we plot $\exp[4(S_L^{(2)}-S_{N/2}^{(2)})/c]$ for $N=200$ and several values of α. For a CFT with central charge $c=1$ one expects this quantity to be $\sin(\pi L/N)$,[5] which is also plotted (dashed line). The numerical results agree (in average) very well with this prediction, confirming the criticality of the iMPS for $\alpha\leq 1/2$. Note that the oscillations are not a feature of the numerical

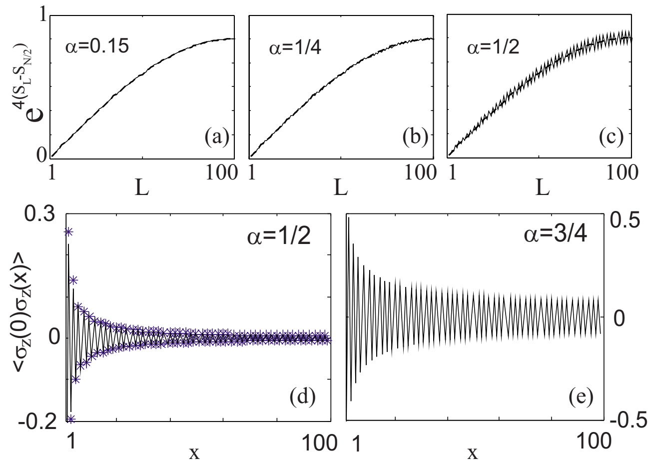

FIG. 2. (Color online) [(a)–(c)] Renyi entropy $S_L^{(2)}$ for a chain with $N=200$ sites and several values of $\alpha \in (0,1/2]$. The dashed line shows the CFT prediction for $c=1$. [(d) and (e)] Correlator C_n^{zz} for several values of α. In (d) the stars indicate the exact result.

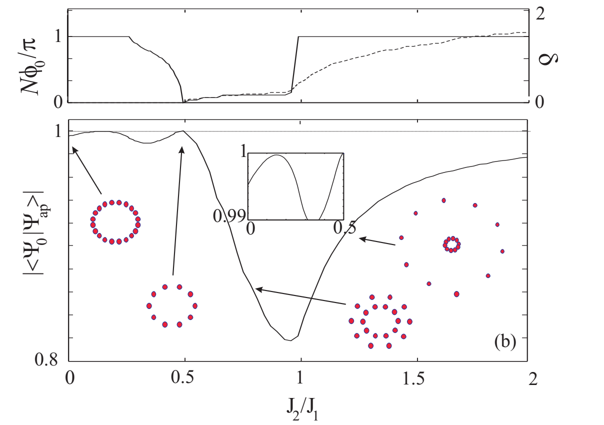

FIG. 3. (Color) J_1-J_2 model (a) values of ϕ_0 and δ for which the energy is minimal; (b) overlap of the iMPS state with the exact GS. The values of the z_n in the complex plane are qualitatively depicted for each region.

calculations but they are intrinsic in the model. For $\alpha > 1/2$, we have checked that the Renyi entropy saturates to a constant value independent of L, in accordance with the gapped character of the XXZ spin chain with $\Delta > 1$.

Other quantities that can be easily computed using Monte Carlo techniques are spin-spin correlators $C_n^{aa} = \langle \sigma_n^a \sigma_0^a \rangle (a = x,y,z)$. Figures 2(d) and 2(e) shows the correlator C_n^{zz} for $\alpha = 1/2, 3/4$. In the case $\alpha = 3/4$, the correlator exhibits antiferromagnetic long-range order, as expected for the gapped $\Delta > 1$ regime. For $\alpha = 1/2$ we can compare with the exact result (stars in the figure) $C_n^{zz} = (-1)^n \mathrm{Si}(\pi n)/(\pi n)$, where $\mathrm{Si}(x)$ is the sine integral function. For this value of α, the system is isotropic (see below), so C_n^{aa} is independent of a, and its expression was first obtained from a Gutzwiller projection of the one-band Fermi state.[14] This result motivated Haldane and Shastry to construct their inverse square exchange Hamiltonian.[10] These authors also noticed that C_n^{xx} coincides with the one-body density matrix of the Calogero-Sutherland model of a gas of hard-core bosons.[11] The GS of the latter model is a continuum version of Eq. (6) for $\alpha = 1/2$. For other values of $\alpha \in (0,1/2]$, the asymptotic behavior of the one-body density-matrix correlator is $C_n^{xx} \sim n^{-2\alpha}$,[15] which can be compared with the exact scaling in the critical XXZ model $C_n^{xx} \sim n^{-\eta} (\Delta = -\cos \pi \eta)$.[16] The comparison of these two results yields, $\Delta = -\cos(2\pi\alpha)$, which correctly reproduces the cases: $\alpha = 0, 1/4, 1/2$ [see Fig. 1(b)].

(2) *J_1-J_2 Heisenberg model*. We use the iMPS ansatz for this frustrated antiferromagnet model described by the Hamiltonian

$$H_{J_1,J_2} = \sum_{i=1}^{N} (J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_i \cdot \mathbf{S}_{i+2}). \tag{10}$$

The phases of this model are: (i) critical $c=1$ phase $(0 \le J_2 \le J_{2,c} \sim 0.241$, (ii) spontaneously dimerized phase $(J_{2,c} < J_2 \le J_{\mathrm{MG}} = 0.5)$, and (iii) incommensurate spiral phase $(J_2 > J_{\mathrm{MG}})$.[17] J_{MG} is the Majumdar-Gosh point whose two GS are the dimer configurations. Since this model is isotropic we shall choose the ansatz, Eq. (4), with $\alpha = 1/2$ (see Ref. 18 for a related ansatz). For the choice of the z_i parameters we distinguish between even and odd sites

$$z_{2n} = e^{\delta - i\phi_0 + 4\pi i n/N}, \quad z_{2n+1} = e^{-\delta + i\phi_0 + 4\pi i n/N}, \quad n = 1, \ldots, \frac{N}{2},$$

where $\phi_0 \in [0, \pi/N]$ and δ are variational parameters, which for a translational invariant state are $(\phi_0, \delta) = (\pi/N, 0)$. These parameters are found minimizing the energy, and their value (a) as well as the overlap with the exact GS wave function (b) are shown in Fig. 3 as functions of J_2/J_1. At $J_2 \sim J_{2,c}$, the parameter ϕ_0 departures from π/N, which reflects the spontaneous dimerization of the system. At the MG point, $\phi_0 = \delta = 0$ and the iMPS is a linear combination of the dimer states. For $J_2 > J_{\mathrm{MG}}$ the parameter δ deviates from zero. Finally, at $J_2/J_1 \sim 1$, one finds $\delta = \pi/N$, while δ increases steadily with an overlap approaching one, meaning that the two chains become increasingly decoupled. A pictorial rep-

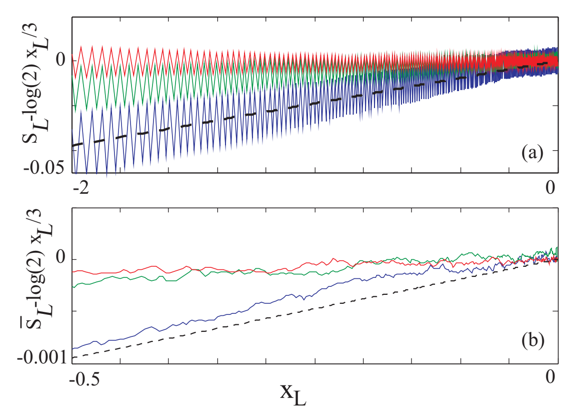

FIG. 4. (Color) Renyi entropy $S_L^{(2)}$ as a function of $x_L = \log[\sin(\pi L/N)]$. We have subtracted from the entropy $\log(2) x_L/3$ in order to compare with the prediction (Refs. 20 and 21). Upper (red), medium (green), and lower (blue) curves correspond to $\delta = 0.75, 0.5, 0.1$. The dashed line corresponds to $x_L/4$. In (b) we have averaged over consecutive points and plotted for low values of x_L.

resentation of the variational parameters is also shown in Fig. 3(b).

(3) *Inhomogeneous Haldane-Shastry model.* Each (finite) MPS is the GS of a finite range parent (frustration free) Hamiltonian.[2] Hence one may expect the iMPS parent Hamiltonians to have a range comparable to the size of the system. We will show that this is the case for $\alpha=1/2$ and arbitrary z_n. Remarkably, the corresponding parent Hamiltonian has two-spin interactions only and is a generalization of the HS model. First notice that the wave function (4) is the chiral conformal block of N primary fields, of spin 1/2 and conformal weight $h=1/4$, in the $SU(2)_1$ WZW model. These primary fields are nothing but the chiral vertex operators, Eq. (3), for $\alpha=1/2$. The chiral conformal blocks of the $SU(2)_k$ WZW model, on a cylinder, satisfy the Knizhnik-Zamolodchikov equations,

$$\left(\frac{k+2}{2}z_i\frac{\partial}{\partial z_i}-\sum_{j\neq i}\frac{z_i+z_j}{z_i-z_j}\mathbf{S}_i\cdot\mathbf{S}_j\right)\psi_{\rm cyl}(\mathbf{z})=0, \qquad (11)$$

where $\psi_{\rm cyl}(\mathbf{z})=\Pi_i^N z_i^{1/4}\psi(\mathbf{z})$ is a conformal transformation of the wave function (4) from the complex plane into the cylinder. Now, using Eq. (11), for $k=1$, and Eq. (4) one can prove that $\psi_{\rm cyl}(\mathbf{z})$ is an eigenstate of the Hamiltonian

$$H=-\sum_{i\neq j}\left[\frac{z_iz_j}{(z_i-z_j)^2}+\frac{w_{ij}(c_i-c_j)}{12}\right]\mathbf{S}_i\cdot\mathbf{S}_j \qquad (12)$$

with eigenenergy

$$E=\frac{1}{16}\sum_{i\neq j}w_{ij}^2-\frac{N(N+1)}{16}, \qquad (13)$$

where $w_{ij}=(z_i+z_j)/(z_i-z_j), c_i=\Sigma_{j\neq i}w_{ij}$. Taking $z_n=e^{2\pi i n/N}$, the parameters c_i vanish and Eq. (12) becomes the HS Hamiltonian whose GS is indeed Eq. (5). For other choices of z_n, we have checked numerically that $\psi_{\rm cyl}$ is the GS of Eq. (12). Hamiltonian (12) is an inhomogeneous generalization of the HS model. The uniform HS model has a huge degeneracy in the spectrum that can be explained by a Yangian symmetry. This degeneracy is broken in the nonuniform case.

We can use the above construction to study the entanglement entropy of random models. The scaling of the von Neumann entropy for the random antiferromagnetic Heisenberg model (AFH) model is $\frac{1}{3}\log 2\log L$,[19] and it is conjectured that the same law holds for the Renyi entropy.[20,21] We take the iMPS ansatz, Eq. (4), with $\alpha=1/2$ and $z_n=e^{2\pi i(n+\phi_n)/N}$, and random choices of ϕ_n uniformly distributed in $[-\delta/2,\delta/2]$. This corresponds to having the inhomogeneous HS model with random couplings. We have computed $S_L^{(2)}$ averaged over realizations and plotted it in Fig. 4 for $N=1000$. We have subtracted $\frac{1}{3}\log 2\log L$ to compare with the prediction[20,21] which should yield a horizontal line at 0. For $\delta=0.75,0.5$, if we ignore the oscillations, we find a very good agreement. Even though for $\delta=0.1$ the result seems to fit better with the formula $\frac{1}{4}\log L$, the inset shows that for long distances the previous result seems to apply. Thus, the larger the δ the more valid the prediction is for shorter blocks.

In this paper we have proposed an infinite-dimensional version of the MPS using the chiral vertex operators of a $c=1$ CFT, which leads variational wave functions of the Jastrow form. This generalization allow us to study the entanglement properties and correlators of critical and noncritical spin chains. For isotropic spin chains the CFT is the $SU(2)_1$ WZW model and this fact allow us to construct their associated parent Hamiltonians. They are given by an inhomogeneous generalization of the Haldane-Shastry Hamiltonian. Elsewhere it will be shown how to construct models based on the $SU(2)_k$ WZW model for $k>1$, whose conformal blocks yield degenerate ground states.[22]

We thank P. Calabrese and M. Hastings for useful discussions. This work was supported by the projects FIS2006-04885, EU STREP (Quevadis), DFG (FOR635), and by the ESF INSTANS 2005-2010.

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