Infinite matrix product states, Conformal Field Theory and the Haldane-Shastry model

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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 Renni 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.

In recent years the study of one-dimensional quantum lattice systems has received an enormous impetus due the invention of novel numerical algorithms, like DMRG [1] and its extensions (for a review see [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 towards 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 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 of 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 letter 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 non-critical 1D systems on equal footing. In particular, we will consider the XXZ and J1-J2 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 Jas-trow type wave functions. There exists many important examples of that type wave functions, such as the Laugh-lin of the FQHE [9], the Haldane-Shastry 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 Haldane-Shastry (HS) wave function. This case is particularly interesting because there is an enhanced symmetry described by the $SU(2)$ Wess-Zumino-Witten model at level 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 [20, 21].

Let us consider a spin-1/2 chain with $N$ sites, and local spin basis $|s_i\rangle$, where $s_i = \pm1$ $(i = 1, \ldots, N)$. A generic state in the Hilbert space of this spin chain is given by

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

A MPS state is an ansatz of the form

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

where $A_{s_i}^{(i)}$ 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 $2^N$, which is much smaller than the number of components of a generic state $|\psi\rangle$, namely $2^N$. To define a IMPS we shall replace the matrices $A_{s_i}^{(i)}$ 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

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

where $z_i$ are complex numbers, $\alpha$ a positive real number and $\chi_{s_i} = 1, s_i$ for $i$ even and odd respectively [13]. 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

\[ \psi(s_1, \ldots, s_N) = \delta_s e^{i\pi/2 S_{\text{odd}}} \prod_{i>j} (z_i - z_j)^{\alpha s_i s_j} \]  

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 \( \delta_s \) to the local spin \( s_i \), so that the total third component of the spin, \( S^z = \sum_i s_i^z/2 \), vanishes. We will use the IMPS variationally, with \( z_i \) and \( \alpha \) as variational parameters. The wave function scales with an overall factor under a Moebius transformation \( z_i \rightarrow (az_i + b)/(cz_i + d) \) \( \forall i \), 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 \( z_n = e^{i\pi n/N} \) \((n = 1, \ldots, N)\). In that case we have

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

For later purposes, it is convenient to express this spin wave function using hard-core boson variables. Mapping the spin up (down) states into empty (occupied) hard-core boson states, one finds

\[ \psi(n_1, \ldots, n_{N/2}) \propto e^{i\pi \sum_n n_{i=1}^{N/2} \left( \frac{\sin \pi (n_i - n_j)}{N} \right)^{4\alpha}} \]  

where \( n_i = 1, \ldots, N \) denote the positions of \( N/2 \) hard-core bosons in the lattice.

1. The XXZ spin chain: The Hamiltonian with anisotropic coupling \( \Delta \) is given by

\[ H_{\text{XXZ}} = \sum_{i=1}^N \left( S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z \right) \]  

where \( S_{N+1} = S_1 \) for periodic boundary conditions (we take \( N \) to be even). This model displays three different phases at zero temperature: i) a gapped 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 \( |0\rangle \), which favours antiparallel nearest-neighbour spins. We expect this ansatz to adequately describe the \( \Delta > -1 \) regimes. The only variational parameter left in \( |0\rangle \) is \( \alpha \), which we fix by numerically minimizing the energy. In Fig. we plot this overlap as a function of \( \Delta \), 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 \( \alpha = 0 \) and 1/4 respectively. This indicates that the corresponding IMPS states coincide with the exact GS. To prove this result, one applies the unitary transformation \( U = \prod_{\text{odd}} (2S_i^z) \) to \( |0\rangle \) 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 \( \alpha \) for \( \alpha = 0 \). 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

\[ f(n_1, \ldots, n_{N/2}) \propto \prod_{n_i>n_j} \frac{\sin \pi (n_i - n_j)}{N} \]  

where \( n_1, \ldots, n_{N/2} \) are the positions of the bosons on the lattice. Undoing the \( U \) transformation, one recovers the state \( |0\rangle \), with \( \alpha = 1/4 \). For the isotropic XXX model, \( \Delta = 1 \), the maximal overlap is obtained for \( \alpha = 1/2 \). The corresponding wave function \( |0\rangle \) does not yield the exact GS, but its hard-core version \( \alpha \) coincides with the GS of the Halldane-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 IMP ansatz \( |0\rangle \), 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

\[ S_2^{(2)} = -\log \rho_{2} \]  

where \( \rho_{2} \) is the density matrix of \( |0\rangle \) restricted to a subsystem of size \( L \). The computation is performed as follows. We rewrite

\[ e^{-S_2^{(2)}} = \sum_{n,m,n',m'} |\langle n,m|\psi\rangle|^2 |\langle n',m'|\psi\rangle|^2 \frac{\langle \psi|n',m'\rangle \langle \psi|n,m\rangle}{\langle \psi|n,m\rangle \langle \psi|n',m'\rangle} \]  

where \( |n\rangle \) (and \( |n'\rangle \)) is an orthonormal basis in the space of the \( L \) spins, and \( |n\rangle \) (and \( |n'\rangle \)) another corresponding to the rest of spins. This expression can be easily evaluated by using two independent spin chains and performing the additions using MonteCarlo techniques. In Fig.
we plot \( \exp[4(S_1^{(2)} - S_{N/2}^{(2)})/c] \) for \( N = 200 \) and several values of \( \alpha \). For a CFT with central charge \( c = 1 \) one expects this quantity to be \( \sin(\pi L/N) \) [2], 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 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 \( \Delta > 1 \).

Another quantities that can be easily computed using MonteCarlo techniques are spin-spin correlators \( C_{n}^{\alpha a} = \langle \sigma_{n}^{\alpha} \sigma_{n}^{a} \rangle \) \( (a = x, y, z) \). Fig.2(d,e) shows the correlator \( C_{n}^{zz} \) for \( \alpha = 1/2, 3/4 \). In the case \( \alpha = 3/4 \), the correlator exhibits anti-ferromagnetic 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) \( C_{n}^{zz} = (-1)^{n/2} \sin(n\pi)/n \) which is the sine integral function. For this value of \( \alpha \), the system is isotropic (see below), so \( C_{n}^{aa} \) is independent of \( a \), and its expression was first obtained from a Gutwiller 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 (9) for \( \alpha = 1/2 \). For other values of \( \alpha \in (0,1/2) \), the asymptotic behaviour 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 \( C_{n}^{xx} \sim n^{-\eta} (\Delta = -\cos(\pi \alpha)) \) [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. 3(b)).

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

\[
H_{J_1,J_2} = \sum_{i=1}^{N} (J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_i \cdot \mathbf{S}_{i+2})
\]

![FIG. 3: J₁–J₂ model (a) Values of φ₀ 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.](image)

The phases of this model are: i) critical \( c = 1 \) phase \((0 \leq J_2 \leq J_{2,c} = 0.241) \), ii) spontaneously dimerized phase \((J_{2,c} < J_2 \leq J_{MG} = 0.5) \) and iii) incommensurate spiral phase \((J_2 > J_{MG}) \) [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 [3] with \( \alpha = 1/2 \) (see [18] for a related ansatz). For the choice of the \( z_i \) parameters we distinguish between even and odd sites

\[
z_{2n} = e^{δ - iφ_0 + \frac{4δn}{N}}, \quad z_{2n+1} = e^{-δ + iφ_0 + \frac{4δn}{N}}, \quad n = 1, \ldots, \frac{N}{2}
\]

where \( φ_0 \in [0, \pi/N] \) and \( δ \) are variational parameters, which for a translational invariant state are \((φ_0, δ) = (π/N, 0) \). 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 \( φ_0 \) departs from \( \pi/N \), which reflects the spontaneous dimerization of the system. At the MG point, \( φ_0 = δ = 0 \) and the IMPS is a linear combination of the dimer states. For \( J_2 > J_{MG} \) the parameter \( δ \) departs from zero. Finally, at \( J_2/J_1 \sim 1 \), one finds \( δ = π/N \), while \( δ \) increases steadily with an overlap approaching one, meaning that the two chains become increasingly decoupled. A pictorial representation 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 the case $\alpha = 1/2$ 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 transformation of the wave function [3] from the complex plane into the cylinder. Now, using eqs (11) and (4) one can prove that $\psi_{cyl}(z)$ is an eigenstate of the Hamiltonian

$$H = -\sum_{ij} \left( \frac{z_i z_j}{(z_i - z_j)^2} + \frac{w_{ij}(c_i - c_j)}{12} \right) S_i \cdot S_j$$

(12)

with eigenenergy

$$E = \frac{1}{16} \sum_{ij} w_{ij}^2 - \frac{N(N+1)}{16}$$

(13)

where $w_{ij} = (z_i + z_j)/(z_i - z_j), c_i = \sum_{j \neq i} w_{ij}$. Taking $z_n = e^{2\pi n/N}$, the parameters $c_i$ vanish and (12) becomes the HS Hamiltonian whose GS is indeed (5). For other choices of $z_n$, we have checked numerically that $\psi_{cyl}$ is the GS of (12). The Hamiltonian (12) is an inhomogeneous generalization of the HS model, which seems to be integrable due to the existence of higher conserved quantities that can be derived from the KZ equation (11). 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 non uniform 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 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 (4) with $\alpha = 1/2$ and $z_n = e^{2\pi i (n+\phi_n)/N}$, and random choices of $\phi_n$ 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. (a) for $N = 1000$. We have subtracted $\frac{1}{4} \log 2 \log L$ 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 $\frac{1}{3} \log L$, the inset shows that for long distances the previous result seems to apply. Thus, the larger the $\delta$ the more valid the prediction is for shorter blocks.

FIG. 4: 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 [20] [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 $x_L$.

In this letter we have proposed an infinite dimensional version of the MPS using the chiral vertex operators of a $c = 1$ CFT. This generalization allow us to study the entanglement properties and correlators of critical and non critical 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 inhomogenous generalization of the Haldane-Shastry Hamiltonian, that seems to be integrable. Our construction can be generalized in principle to any CFT. For rational CFTs, such as the WZW models, we expect that the conformal blocks may provide degenerate GS with non-abelian statistics encoded in their braiding matrices.

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