Accurate Determination of Tensor Network State of Quantum Lattice Models in Two Dimensions

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We have proposed a novel numerical method to calculate accurately physical quantities of the ground state using the tensor network wave function in two dimensions. The tensor network wave function is determined by an iterative projection approach which uses the Trotter-Suzuki decomposition formula of quantum operators and the singular value decomposition of matrix. The norm of the wave function and the expectation value of any physical observable are evaluated by a coarse-grain tensor renormalization group approach. Our method allows a tensor network wave function with a high bond degree of freedom (such as \( D = 8 \)) to be handled accurately and efficiently in the thermodynamic limit. For the Heisenberg model on a honeycomb lattice, our results for the ground state energy and the staggered magnetization agree well with those obtained by the quantum Monte Carlo and other approaches.

Below we will take the \( S = 1/2 \) Heisenberg model on a honeycomb lattice as an example to show how the method works. The Hamiltonian is defined by

\[
H = \sum_{\langle ij \rangle} H_{ij},
\]

\[
H_{ij} = J S_i S_j - \frac{1}{2} h \left( (-)^{S_i z} + (-1)^{S_j z} \right),
\]

where \( \langle ij \rangle \) stands for summation over nearest neighboring sites and \( h \) is the magnitude of a staggered magnetic field. It is straightforward to extend the method to other quantum lattice models with short range interactions in two dimensions.

As the Hamiltonian is translational invariant, we assume the tensor network state to have the following form:

\[
|\Psi\rangle = \text{Tr} \prod_{i \in h, j \in w} \lambda_{x_i y_i z_i} A_{x_i y_i z_i} [m_i] B_{x_i y_i z_i} [m_j] m_i m_j.
\]

A schematic representation of this tensor network state is shown in Fig. 1. In Eq. (3) \( b \) (\( w \)) stands for the black (white) sublattice. \( m_j \) is the eigenvalue of \( S_i z \). \( A_{x_i y_i z_i} [m_i] \) and \( B_{x_i y_i z_i} [m_j] \) are the two three-indexed tensors defined on the black and white sublattices, respectively. \( \lambda_{x_i y_i z_i} \) (\( \alpha = x, y, z \)) are positive diagonal matrices (or vectors) of dimension \( D \) defined on the bond emitted from site \( i \) along the \( \alpha \) direction. The subscripts \( x_i, y_i, \) and \( z_i \) are the integer bond indices of dimension \( D \) (i.e., each running from 1 to \( D \)). A bond links two sites. The two bond indices defined from the two end points take the same values. For example, if the bond connecting \( i \) and \( j \) along the \( x \) direction, then \( x_i = x_j \). The trace is to sum over all spin configurations \( \{ \ldots, m_i, m_j, \ldots \} \) and over all bond indices.

The ground state wave function can be determined by applying the projection operator \( \exp(-\tau H) \) to an arbitrary
From this, applying the Trotter-Suzuki formula, we can express the direction only. These terms commute with each other. By using exp(\(-\tau \hat{H}_a\)), we can express the projection operator as

\[ e^{-\tau \hat{H}} = e^{-\tau \hat{H}_x} e^{-\tau \hat{H}_y} e^{-\tau \hat{H}_z} + o(\tau^2). \] (4)

This means that each iteration of projection can be done using exp(\(-\tau \hat{H}_a\)) (\(\alpha = x, y, z\)) in three separate steps. In the first step, the projection is done with \(\hat{H}_x\). As only two neighboring spins connected by horizontal bonds have interactions in \(\hat{H}_x\), the resulting projected wave function can be expressed as

\[ e^{-\tau \hat{H}_x} |\Psi\rangle = \text{Tr} \prod_{i\in \text{black}} \sum_{m_1} \langle m_1 | e^{-\tau \hat{H}_{x,y,z}(m_1,m_1)} \lambda_x \lambda_y \lambda_z A_{x,y,z}(m_1) B_{x,y,z}(m_1) |m_1\rangle^\dagger |m_1\rangle. \] (5)

From this, a \((D^2d) \times (D^2d)\) matrix can be defined by

\[ S_{x,y,z,m_1,m_2} = \sum_{m_1} \langle m_1 | e^{-\tau \hat{H}_{x,y,z}} |m_1\rangle \lambda_x \lambda_y \lambda_z A_{x,y,z}(m_1) B_{x,y,z}(m_1) \lambda_y, \lambda_z. \] (6)

where \(d = 2\) is the total number of states of a \(S = 1/2\) spin. Taking the singular value decomposition for this matrix, one can further express this \(S\) matrix as

\[ S_{x,y,z,m_1,m_2} = \sum_x U_{y,z,m_1,x} \tilde{\lambda}_x V_{x,y,z,m_2}^\dagger, \] (7)

where \(U\) and \(V\) are two unitary matrices and \(\tilde{\lambda}_x\) is a positive diagonal matrix of dimension \(D^2d\).

Next we truncate the basis space by keeping only \(D\) largest singular values of \(\tilde{\lambda}_x\). Then we set the left \(\tilde{\lambda}_x\) as the new \(\lambda_x\) (\(x = 1, \ldots, D\)) and update the tensors \(A\) and \(B\) by the following formula:

\[ A_{x,y,z}(m_1) = \lambda_{x,y}^{-1} \lambda_{y,z}^{-1} U_{y,z,m_1,x}, \] (8)

\[ B_{x,y,z}(m_1) = \lambda_{y,z}^{-1} \lambda_{z,x}^{-1} V_{x,y,z,m_1,x}. \] (9)

A flow chart of the above one-step renormalization of the wave function is shown in Fig. 2. The next two steps of projections can be similarly done with \(\hat{H}_y\) and \(\hat{H}_z\), respectively. This completes one iteration of the projection. By repeating this iteration procedure many times, an accurate ground state wave function can then be projected out. This iteration process is very efficient. The converging speed depends on the truncation error. In our calculation, we take \(\tau = 10^{-3}\) initially and then gradually reduce it to \(10^{-5}\) to ensure the convergence of the wave function. The number

![FIG. 1. Schematic representation of a tensor network state on a honeycomb lattice. The lattice is divided into two sublattices, represented by the black and white dots, respectively. Each vertex, on which a spin state is inhibited, is connected with three neighboring vertices along three directions, labeled by \(x\), \(y\), and \(z\). On each bond, there is a diagonal matrix (or a vector), \(\lambda_{x,y,z}\), where the subscript \(x = x, y, z\) is a bond index of dimension \(D\). At each vertex, a tensor representation of the spin state \(m\), \(\lambda_{x,y,z}(m)\) for the black sublattice or \(B_{x,y,z}(m)\) for the white sublattice, is defined. A tensor network state is a product of all these bond vectors and vertex tensors.

![FIG. 2. Flow chart of the one-step renormalization of the wave function. (a) To use \(\exp(-\hat{H}_{{\alpha}+}\tau)\) to act on the tensor network state. (b) To evaluate the \(S\) matrix defined by Eq. (6). (c) To perform the singular value decomposition for \(S\). (d) To truncate the basis space of \(\tilde{\lambda}_x\) and to find \(\tilde{A}\) and \(\tilde{B}\) with Eqs. (8) and (9), respectively.]

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We note that both functions. For example, express this matrix as $Tb$.

By taking the singular value decomposition, one can also truncate the basis space and keep only basis states corresponding to the largest singular values of $Tb$.

The above coarse-grain tensor renormalization group method proposed by Levin and Nave [11] to evaluate renormalization group method proposed by Levin and Nave [11] to evaluate $\langle \Psi | \hat{O} | \Psi \rangle$ and $\langle \Psi | \hat{O} | \Psi \rangle$ are tensor network functions. For example,

$$\langle \Psi | \hat{O} | \Psi \rangle = \text{Tr} \sum_{i\in b, j\in e} T^a_{i,x,y,z} T^b_{j,x',y',z'}$$

where the trace is to sum over all bond indices. Both $T^a$ and $T^b$ are $D^2 \times D^2 \times D^2$ tensors. $T^a$ is defined by

$$T^a_{x,y,z} = \sum \left( \lambda x y z \right)^{1/2} A_{x,y,z} \left[ m \right] A_{x',y',z'} \left[ m \right] \left( \lambda x ' y ' z ' \right)^{1/2}.$$  

(12)

$T^b$ is similarly defined. Thus we can apply the tensor renormalization group method proposed by Levin and Nave [11] to evaluate $\langle \Psi | \hat{O} | \Psi \rangle$ and $\langle \Psi | \hat{O} | \Psi \rangle$.

To perform the tensor renormalization, we first take two $T^a$ and $T^b$ on the two ends of a bond and define the following $D^4 \times D^4$ matrix:

$$M_{l',kk'} = \sum_{n} T^a_{l'n,k} T^b_{nk'l'}.$$  

(13)

By taking the singular value decomposition, one can also express this matrix as

$$M_{l',kk'} = \sum_{n=1,...,D^4} U_{l'n,n} \Lambda_n V_{kk'n}.$$  

(14)

where $U$ and $V$ are unitary matrices, $\Lambda_n$ is a positive defined diagonal matrix of dimension $D^4$. Again we will truncate the basis space and keep only basis states corresponding to the largest $D^2$ singular values of $\Lambda$. Then the $M$ matrix can be approximately expressed as

$$M_{l',kk'} = \sum_{n=1,...,D^2} S^a_{nll'} S^b_{nk'}.$$  

(15)

where

$$S^a_{nll'} = \sqrt{\Lambda_n U_{ll',n}}.$$  

(16)

of iterations used in our calculation is generally around 10^5–10^6.

Given $|\Psi\rangle$, the expectation value of a measurable quantity $O$ is defined by

$$\langle \hat{O} \rangle = \langle \Psi | \hat{O} | \Psi \rangle.$$  

(10)

We note that both $\langle \Psi | \hat{O} | \Psi \rangle$ and $\langle \Psi | \hat{O} | \Psi \rangle$ are tensor network functions. For example,

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We have applied the above approach to the spin-\(\frac{1}{2}\) anti-ferromagnetic Heisenberg model (2). Both ground state energy and the staggered magnetization \(M\) defined by

\[ M(h) = \frac{E(h) - E(0)}{h} \quad (20) \]

are calculated. In Eq. (20), \(E(h)\) is the ground state energy in a finite staggered magnetic field \(h\). The lattice size is \(N = 6 \times 3^{10}\). The finite size effect is negligible compared with the truncation error in the tensor renormalization.

Table I shows the ground state energy and the staggered magnetization as a function of \(D\) for the Heisenberg model with \(h = 0\). The zero field staggered magnetization is obtained by extrapolating \(M(h)\) obtained at finite \(h\) (Fig. 5) to the limit \(h \to 0\). With \(D = 8\), we find that the ground state energy \(E = -0.5506\) and the staggered magnetization \(M = 0.21 \pm 0.01\) in the zero field limit. They agree well with results obtained by other approaches (see Table II).

In conclusion, we have proposed a novel method to treat the tensor network wave function of quantum lattice models in two dimensions. It allows us to determine the tensor network wave function of the ground state accurately and efficiently. The ground state energy and the staggered magnetization of the \(S = 1/2\) Heisenberg model on the honeycomb lattice obtained with this method are consistent with those obtained by other methods. By fully considering the symmetry of the Hamiltonian, we believe that a larger local tensor with \(D \sim 20\) can be accessed with our method.

This can further improve the accuracy of results and make this method even more powerful.

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TABLE II. Comparison of our results with those obtained by other approaches for the ground state energy per site \(E\) and the staggered magnetization \(M\) of the Heisenberg model with \(h = 0\).

<table>
<thead>
<tr>
<th>Method</th>
<th>(E)</th>
<th>(M)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spin wave [12]</td>
<td>-0.5489</td>
<td>0.24</td>
</tr>
<tr>
<td>Series expansion [13]</td>
<td>-0.5443</td>
<td>0.27</td>
</tr>
<tr>
<td>Monte Carlo [14]</td>
<td>-0.5450</td>
<td>0.22</td>
</tr>
<tr>
<td>Ours (D = 8)</td>
<td>-0.5506</td>
<td>0.21 ± 0.01</td>
</tr>
</tbody>
</table>