Accurate determination of tensor network state of quantum lattice models in two dimensions

H. C. Jiang, Z. Y. Weng, and T. Xiang
1Center for Advanced Study, Tsinghua University, Beijing, 100084, China
2Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100190, China
3Institute of Theoretical Physics, Chinese Academy of Sciences, P.O. Box 2735, Beijing 100190, China

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We have proposed a novel numerical method to calculate accurately the physical quantities of the ground state with the tensor-network wave function in two dimensions. We determine the tensor network wavefunction by a projection approach which applies iteratively the Trotter-Suzuki decomposition of the projection operator and the singular value decomposition of matrix. The norm of the wavefunction and the expectation value of a physical observable are evaluated by a coarse grain renormalization group approach. Our method allows a tensor-network wavefunction 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.

We will generalize the classic coarse grain renormalization group approach proposed by Levin and Nave \(^{11}\) to the quantum system, and use it to calculate the norm of the wave function and the expectation value of any physical observable. This provides an accurate and efficient tool to determine the expectation values of physical quantities from the tensor-network wavefunction of the ground state.

Below, we will take the S=1/2 Heisenberg model on a honeycomb lattice

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

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

as an example to show how the method works. Here, \( \langle ij \rangle \) means that \( i \) and \( j \) are the two nearest neighboring sites, \( h \) 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. We assume the tensor network state to have the following form

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

A schematic representation of this tensor network state is shown in Fig. 1. In Eq. \( \lambda_{x,y,z} \) stands for the black/white sublattice. \( m_i \) is the eigenvalue of \( S_{i,z} \). \( A_{x_i,y_i,z_i}[m_i] \) and \( B_{x_j,y_j,z_j}[m_j] \) are the two three-indexed tensors defined on the black and white sublattices, respectively. \( \lambda_{\alpha} \) (\( \alpha = x, y, z \)) is a 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 \( \{ \cdots, m_i, m_j, \cdots \} \) and over all bond indices.
The ground state wavefunction can be determined by applying the projection operator \( \exp(-\tau H) \) to an arbitrary initial state |\( \Psi \rangle \). In the limit \( \beta \to \infty \), \( \exp(-\tau H)|\Psi \rangle \) will converge to the ground state of \( H \). However, this projection cannot be done in a single step since the terms in \( H \) defined by Eq. (2) do not commute with each other. In real calculation, we will take a small \( \tau \) and apply this projection operator to |\( \Psi \rangle \) iteratively for many times.

Let us start by dividing the Hamiltonian into three parts

\[
H = H_x + H_y + H_z,
\]

\[
H_\alpha = \sum_{i \in \text{black}} H_{i,i+\alpha} \quad (\alpha = x, y, z).
\]

\( H_\alpha \) (\( \alpha = x, y, z \)) contains all the interaction terms along the \( \alpha \)-direction only. These terms commute with each other. From the Suzuki-Trotter formula, we can then express the projection operator as

\[
e^{-\tau H} \approx e^{-\tau H_x} e^{-\tau H_y} e^{-\tau H_z} + o(\tau^2).
\]

This means that each iteration of projection can be done using \( \exp(-\tau H_\alpha) \) (\( \alpha = x, y, z \)) in three separate steps.

In the first step, the projection is done with \( H_x \). As only the two neighboring spins connected by horizontal bonds have interactions in \( H_x \), the resulting projected wavefunction can expressed as

\[
e^{-\tau H_x}|\Psi\rangle = \prod_{i\in b,j\in w} \sum_{m_i,m_j} \langle m'_i|m'_j|e^{-H_{ij}}|m_i,m_j\rangle \lambda_{x,i} \lambda_{y,i} \lambda_{z,i} A_{x,y,z}[m_i] B_{x,y,z}[m_j] |m'_i,m'_j\rangle.
\]

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

\[
S_{y,z,m_i'y,z'} = \sum_{m_i,m_j} \langle m'_i|m'_j|e^{-H_{ij}}|m_i,m_j\rangle \lambda_{y,i} \lambda_{z,i} A_{y,z}[m_i] B_{y,z}[m_j] \lambda_{y,j} \lambda_{z,j},
\]

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

\[
S_{y,z,m_i'y,z'} = \sum_x U_{y,z,m_i,x} \hat{\lambda}_x V_{y,z,m_j,x}^T
\]

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

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

\[
A_{x,y,z}[m_i] = \lambda_{y,i} \lambda_{z,i} U_{y,z,m_i,x},
\]

\[
B_{x,y,z}[m_j] = \lambda_{y,j} \lambda_{z,j} V_{y,z,m_j,x}.
\]

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 \( H_y \) and \( H_z \), 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 \( \sim 10^{-5} \) to ensure the convergence of the wavefunction. The number of iterations used in our calculation is generally around \( 10^5 \sim 10^6 \).

Given \(|\Psi\rangle\), the expectation value of a measurement quantity \( \hat{O} \) is defined by

\[
\langle \hat{O} \rangle = \frac{\langle \Psi|\hat{O}|\Psi \rangle}{\langle \Psi|\Psi \rangle}.
\]

We notice that both \(|\Psi\rangle\langle \Psi|\) and \(|\Psi\rangle\langle \hat{O}|\Psi \rangle\) are tensor-network functions. For example,

\[
|\Psi\rangle = \prod_{i\in b,j\in w} T^a_{x,x',i',y,i,y',z,z'} T^b_{x,y,z',y',z},
\]

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

\[
T^a_{x,x',y,y',z,z'} = \sum_m \langle \lambda_x \lambda_y \lambda_z \rangle^{1/2} A_{x,y,z}[m] A_{x',y',z'}[m] \langle \lambda'_{x'} \lambda'_{y'} \lambda'_{z'} \rangle^{1/2}.
\]
$T^b$ is similarly defined. Thus we can apply the tensor renormalization group method proposed by Levin et al. \[11\] to evaluate $\langle \hat{O}\vert \Psi \rangle$ and $\langle \Psi \vert \hat{O} \vert \Psi \rangle$.

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

$$M_{ll',kk'} = \sum_n T^a_{nl,k} T^b_{nk,l}. \quad (13)$$

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

$$M_{ll',kk'} = \sum_{n=1}^{D^4} U_{ll',n} \Lambda_n V_{kk',n}, \quad (14)$$

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

$$M_{ll',kk'} \approx \sum_{n=1}^{D^4} S^a_{nl,l'} S^b_{nk,k'}. \quad (15)$$

where

$$S^a_{nl,l'} = \sqrt{\Lambda_n} U_{ll',n}, \quad (16)$$

$$S^b_{nk,k'} = \sqrt{\Lambda_n} V_{kk',n} \quad (17)$$

are the two vertex tensors defined in the new lattice shown in Fig. (3b).

After the above transformation, the lattice structure is changed (Fig. (3b)). Now we replace each smallest triangle by a single lattice point. This introduce a coarse-grained honeycomb lattice with two coarse-grained tensors $T^a$ and $T^b$ defined by

$$\tilde{T}^a_{xyz} = \sum_{ijk} S^a_{xik} S^a_{yji} S^a_{zkj} \quad (18)$$

$$\tilde{T}^b_{xyz} = \sum_{ijk} S^b_{xik} S^b_{yji} S^b_{zkj}. \quad (19)$$

This coarse grain transformation reduces the lattice by a factor of 3 at each iteration. Iterating this procedure, at the end the honeycomb lattice will eventually becomes 6 (Fig. 4). One can then trace out all bond indices to find the norm of the wavefunction.

The above coarse grain tensor renormalization group transformation can be straightforwardly extended to evaluate $\langle \hat{O}\vert \Psi \rangle$. The difference is that $T^a$ and $T^b$ now may become site dependent and their definitions are changed.

We have applied the above approach the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model \[2\]. Both the ground state energy and the staggered magnetization $M$ defined by

$$M(h) = \frac{E(h) - E_0}{\hbar} \quad (20)$$

are calculated. In Eq. (20), $E(h)$ is the ground state energy in a finite staggered magnetic field $\hbar$. The lattice size is $N = 6 \times 3^{10}$. The finite size effect is negligible.
FIG. 5: (color online) The staggered magnetization $M(h)$ as a function of the staggered magnetic field, at different $D$.

tabulated. Compared with the truncation error resulted from the coarse grain 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 $h \rightarrow 0$. 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 the results obtained by the 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 treat a tensor-network state with $D$ as high as 8 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.

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\begin{table}
\centering
\begin{tabular}{|l|l|l|}
\hline
$D$ & $E$ & $M$ \\
\hline
3 & -0.5365 & 0.249 \\
4 & -0.5456 & 0.228 \\
5 & -0.5488 & 0.220 \\
6 & -0.5513 & 0.206 \\
7 & -0.5490 & 0.216 \\
8 & -0.5506 & 0.212 \\
\hline
\end{tabular}
\caption{The ground state energy per site $E$ and the staggered magnetization $M$ in the zero field limit as a function of $D$.}
\end{table}

\begin{table}
\centering
\begin{tabular}{|l|l|l|}
\hline
Method & $E$ & $M$ \\
\hline
Spin wave[12] & -0.5489 & 0.24 \\
Series expansion[13] & -0.5443 & 0.27 \\
Monte Carlo[14] & -0.5450 & 0.22 \\
Ours D=8 & -0.5506 & 0.21 ± 0.01 \\
\hline
\end{tabular}
\caption{Comparison of our results with those obtained by the other approaches for the ground state energy per site $E$ and the staggered magnetization $M$ of the Heisenberg model with $h = 0$.}
\end{table}

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