# 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 a 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.

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The application of the density matrix renormalization group (DMRG) proposed by White [1] has achieved great success in one dimension [2,3]. However, in two dimensions, the application of the DMRG in both real and momentum space [4,5] has been limited only to small lattices. The error resulting from the DMRG truncation increases extremely fast with increasing size of lattice. To resolve this problem, the tensor network state, which is an extension of the matrix product in one dimension [6], was proposed [7,8]. In a tensor network state, the local tensors interact with each other on all directions of the lattice. This leads to two problems in the treatment of the tensor network state. First, it is difficult to determine accurately all elements of local tensors by any variational approach since the total degree of freedom of a local tensor increases exponentially with the dimension of the tensor. Second, it is difficult to calculate the expectation value of any physical observable even if we know the expression of the tensor network wave function, since the number of summations over the basis configurations increases exponentially with the lattice size.

In this Letter, we propose a novel method to handle the tensor network wave function in two dimensions. We will show that the tensor network wave function $|\Psi\rangle$ of the ground state can be accurately determined by applying an iterative projection approach. This approach is similar to the time-evolving block decimation method that was used to determine the matrix product wave function of the ground state in one dimension [9,10]. Then 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 wave function of the ground state.

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

$$H = \sum_{\langle ij \rangle} H_{ij}, \tag{1}$$

$$H_{ij} = JS_iS_j - \tfrac{1}{2}h[(-)^iS_{i,z} + (-1)^jS_{j,z}], \tag{2}$$

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:

$$|\Psi\rangle = \mathrm{Tr} \prod_{i\in b, j\in w} \lambda_{x_i}\lambda_{y_i}\lambda_{z_i}A_{x_iy_iz_i}[m_i]B_{x_jy_jz_i}[m_j]|m_im_j\rangle. \tag{3}$$

A schematic representation of this tensor network state is shown in Fig. 1. In Eq. (3) $b$ ($w$) stands for the black (white) sublattice. $m_i$ is the eigenvalue of $S_{iz}$. $A_{x_iy_iz_i}[m_i]$ and $B_{x_jy_jz_j}[m_j]$ are the two three-indexed tensors defined on the black and white sublattices, respectively. $\lambda_{\alpha_i}$ ($\alpha = x, y, z$) 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

 

initial state $|\Psi\rangle$. In the limit $\tau \to \infty$, $\exp(-\tau H)|\Psi\rangle$ will converge to the ground state of $H$. However, this projection cannot be done in a single step since 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

$$H = H_x + H_y + H_z, \qquad H_\alpha = \sum_{i \in \text{black}} H_{i,i+\alpha} \qquad (\alpha = x, y, z).$$

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

$$e^{-\tau H} \approx e^{-\tau H_z} e^{-\tau H_y} e^{-\tau H_x} + o(\tau^2). \tag{4}$$

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 two neighboring spins connected by horizontal bonds have interactions in $H_x$, the resulting projected wave function can be expressed as

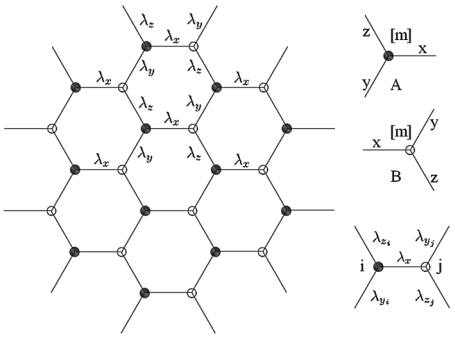


FIG. 1. Schematic representation of a tensor network state on a honeycomb lattice. The lattice is divided into two sublattices, represented by the black and white dots, respectively. Each vertex, on which a spin state is inhibited, is connected with three neighboring vertices along three directions,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

$$e^{-\tau H_x}|\Psi\rangle = \mathrm{Tr} \prod_{i \in b, j=i+x} \sum_{m_i m_j} \langle m_i' m_j' | e^{-H_{ij}\tau} | m_i m_j \rangle \lambda_{x_i} \lambda_{y_i} \lambda_{z_i} A_{x_i y_i z_i}[m_i] B_{x_j y_j z_j}[m_j] | m_i' m_j' \rangle. \tag{5}$$

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

$$S_{y_i z_i m_i', y_j z_j m_j'} = \sum_{m_i m_j} \sum_x \langle m_i' m_j' | e^{-H_{ij}\tau} | m_i m_j \rangle \lambda_{y_i} \lambda_{z_i} A_{x y_i z_i}[m_i] \lambda_x B_{x y_j z_j}[m_j] \lambda_{y_j} \lambda_{z_j}, \tag{6}$$

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

$$S_{y_i z_i m_i, y_j z_j m_j} = \sum_x U_{y_i z_i m_i, x} \tilde{\lambda}_x V^T_{x, y_j z_j m_j}, \tag{7}$$

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

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:

$$A_{x y_i z_i}[m_i] = \lambda_{y_i}^{-1} \lambda_{z_i}^{-1} U_{y_i z_i m_i, x}, \tag{8}$$

$$B_{x y_j z_j}[m_j] = \lambda_{y_j}^{-1} \lambda_{z_j}^{-1} V_{y_j z_j m_j', x}. \tag{9}$$

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 $H_y$ 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 wave function. The number

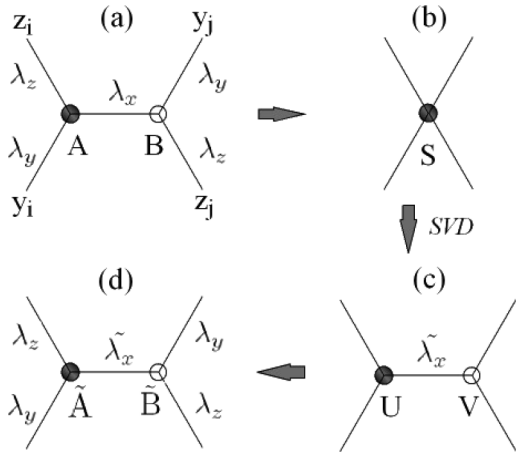


FIG. 2. Flow chart of the one-step renormalization of the wave function. (a) To use $\exp(-H_{i,i+x}\tau)$ to act on the tensor network state. (b) To evaluate the $S$ matrix defined by Eq. (6). (c) To perform the singular value decomposition for $S$. (d) To truncate the basis space of $\tilde{\lambda}_x$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

TABLE I. The ground state energy per site $E$ and the staggered magnetization $M$ in the zero field limit as a function of $D$.

| $D$ | $E$ | $M$ |
|---|---|---|
| 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 |

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

$$\langle \hat{O} \rangle = \frac{\langle \Psi | \hat{O} | \Psi \rangle}{\langle \Psi | \Psi \rangle}. \tag{10}$$

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

$$\langle \Psi | \Psi \rangle = \mathrm{Tr} \prod_{i \in b, j \in w} T^a_{x_i x_i', y_i y_i', z_i z_i'} T^b_{x_j x_j', y_j y_j', z_j z_j'}, \tag{11}$$

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

$$T^a_{xx',yy',zz'} = \sum_m (\lambda_x \lambda_y \lambda_z)^{1/2} A_{xyz}[m] A_{x'y'z'}[m] (\lambda_x' \lambda_y' \lambda_z')^{1/2}. \tag{12}$$

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

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

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

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

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

$$M_{ll',kk'} \approx \sum_{n=1,\ldots,D^2} S^a_{nll'} S^b_{nkk'}, \tag{15}$$

where

$$S^a_{nll'} = \sqrt{\Lambda_n} U_{ll',n}, \tag{16}$$

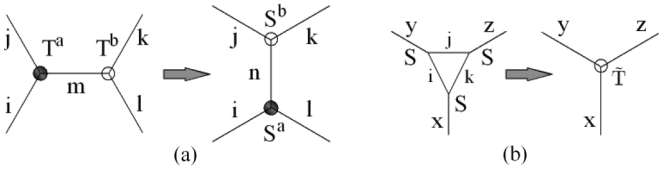


FIG. 3. Steps of coarse graining. (a) Forming the $M$ matrix by tracing out the common bond indices of tensors $T^a$ and $T^b$ defined on the two neighboring sites with Eq. (14), and then perform the singular value decomposition and find two new tensors $S^a$ and $S^b$ defined by Eqs. (16) and (17). (b) Tracing out all common bond indices of $S^a$ tensors (similarly for the $S^b$ tensors) on a triangle formed by the three closed vertices to form a coarse-grained tensor $\tilde{T}^a$ defined by Eq. (18).

$$S^b_{nkk'} = \sqrt{\Lambda_n} V_{kk',n} \tag{17}$$

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

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

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

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

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 be reduced to having only 6 sites (Fig. 4). One can then trace out all bond indices to find the norm of the wave function.

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

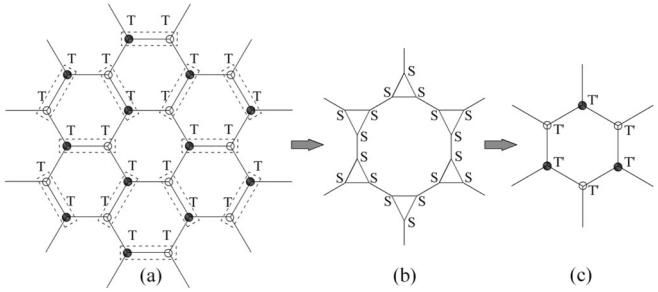


FIG. 4. Tensor renormalization transformation on the honeycomb lattice. (a) The honeycomb lattice. (b) The deformed lattice in the tensor renormalization defined by Eqs. (13)–(15). (c) The squeezed honeycomb lattice after the coarse-grain decimation.

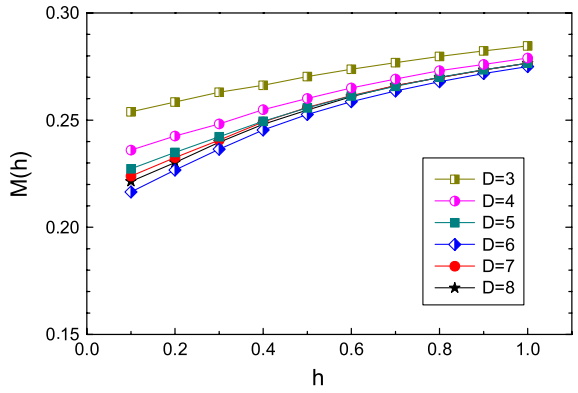


FIG. 5 (color online). The staggered magnetization $M(h)$ as a function of the staggered magnetic field, at different $D$.

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

$$M(h) = \frac{E(h) - E(0)}{h} \tag{20}$$

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.

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 $h = 0$.

| Method | $E$ | $M$ |
|---|---|---|
| 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 | $0.21 \pm 0.01$ |

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

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