Replica exchange molecular dynamics optimization of tensor network states for quantum many-body systems

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Abstract
Tensor network states (TNS) methods combined with the Monte Carlo (MC) technique have been proven a powerful algorithm for simulating quantum many-body systems. However, because the ground state energy is a highly non-linear function of the tensors, it is easy to get stuck in local minima when optimizing the TNS of the simulated physical systems. To overcome this difficulty, we introduce a replica-exchange molecular dynamics optimization algorithm to obtain the TNS ground state, based on the MC sampling technique, by mapping the energy function of the TNS to that of a classical mechanical system. The method is expected to effectively avoid local minima. We make benchmark tests on a 1D Hubbard model based on matrix product states (MPS) and a Heisenberg $J_1-J_2$ model on square lattice based on string bond states (SBS). The results show that the optimization method is robust and efficient compared to the existing results.

Keywords: tensor network, molecular dynamics, optimization, quantum many-body, replica exchange

(Some figures may appear in colour only in the online journal)

1. Introduction

Developing efficient methods to simulate strongly correlated quantum many-body systems is one of the central tasks in modern condensed matter physics. Recently developed tensor network states (TNS) methods, including the matrix product states (MPS) \cite{1–3} and the projected entangled pair states (PEPS) \cite{4}, string bond states (SBS) \cite{5}, multi-scale entanglement renormalization ansatz (MERA) \cite{6} etc provide a promising scheme to solve several long standing quantum many-body problems. In these schemes, the variational space can be represented by some tensors [see equation (1) as an example]. The number of the tensor is polynomially scaled with the number of the sites, and each tensor consists of a set of parameters whose size is determined by the parameter $D$ known as the virtual dimension cut-off. Once we have the TNS representation of the many-particle wave functions, the ground state energies as well as corresponding wave functions can be obtained variationally. However, in practice it is still a great challenge to obtain the ground state of some complicated physical systems (such as frustrated systems and fermionic systems in two dimensions) in the TNS scheme.

Several difficulties reduce the efficiency. The first challenge is polynomial scaling. The computational cost respect to the virtual dimension cut-off $D$, which determines the size of the variational space, is still very high, particularly, in two and higher dimensions. For example, the scaling...
is \(O(D^3)\) for the periodic MPS algorithm [7], \(O(D^\alpha)\) \((8 \leq \alpha \leq 12)\) for the PEPS algorithm [8]. For many important systems, in particular fermionic systems, the parameter \(D\) should be rather large to capture the key physics. However, limited by current computation ability, we can only deal with small \(D\), typically less than 10. To overcome this difficulty, the seminal works, Sandvik et al [9] (based on MPS) and Schuch et al [5] (based on SBS) introduced a Monte Carlo (MC) sampling technique to calculate the physical quantities in tensor networks. Compared to the standard contraction method, the sampling technique reduces dramatically the scaling of computational cost to virtual dimension \(D\). The technique has recently been applied to general TNS, such as PEPS [10]. Based on the MC sampling technique, the MPS scaling can be reduced from \(O(D^5)\) to \(O(D^3)\) for a periodic boundary condition (PBC) [9]. For SBS [5], the scaling is \(O(D^2)\) for a 2D open boundary condition (OBC) system and \(O(D^4)\) for a 2D periodic system with MC sampling technique, which is significantly lower than the standard contraction methods. For a more general PEPS case, the scaling can also be well reduced [10].

Secondly, the energy function is a highly non-linear function of the tensors. With the increasing of \(D\), the parameter space will be larger and the non-linearity of the energy function will increase and its structure will be much more complicated. For frustrated systems, there are a large number of low energy excitations and the gaps between the excited states and the ground states will increase instead of decreasing due to the frustration. For a periodic system, \(E = E_0 + E_0\), where \(E_0\) is the energy of the ground state and \(E_0\) is the energy of the excited state. The low-energy excitation states will appear as the local minima in the energy function. As a result, it is very easy to be trapped in some local minima, when minimizing the energies. As a matter of fact, sometimes when we increase the virtual dimension cut-off \(D\), the ground state energy will increase instead of decreasing due to the trapping to the local minima. Here, we focus on overcoming this difficulty.

In this work, we develop an efficient algorithm to obtain the ground state energy as well as wave function of a TNS based on the MC sampling method. We map the quantum many-particle problem to a classical mechanical problem, in which we treat the tensor elements as the generalized coordinates of the system. We optimize the energy of the system using a replica exchange molecular dynamics method [12, 13]. By exchanging the system configurations among higher and lower temperatures, it can explore large phase space and therefore effectively avoid being stuck in the local minima. The replica exchange method has proven very successful in treating classical spin glass [14] and frustrated spin systems [15] which also suffer from the local minima problem. It also has been successfully used to optimize other highly non-linear problems, such as the three-tangle of general mixed states [16]. Here, we introduce this method in the TNS scheme for quantum many-body systems. We make benchmark tests of the method for a 1D Hubbard model [17] using MPS and the 2D \(J_1-J_2\) Heisenberg model using SBS [18]. The results show improvement over the existing calculations. It is also worth emphasizing that the method introduced here is not limited to the special type of TNS, but applies to general TNS [10].

2. Methods

For simplicity, we describe our method using the example of the MPS type of wave function. The method can be easily generalized to other types of TNS, e.g. SBS [5] and PEPS [10]. The many-particle wave functions of one dimensional periodic systems with \(N\) sites, can be written in the MPS [3], i.e.

\[
|\Psi_{\text{MPS}}\rangle = \sum_{s_1 \ldots s_N = 1}^d \text{Tr}(A^{s_1}_1 A^{s_2}_2 \cdots A^{s_N}_N) |s_1 \cdots s_N\rangle. \tag{1}
\]

where \(d\) is the dimension of the physical indices \(s_k\). \(A^{s_k}_k\) are \(D \times D\) matrices on site \(k\), where \(D\) is the virtual dimension cut-off which determines the size of the variational space.

Given a Hamiltonian \(H\) for a system, the total energy of this system is a function of the tensors at each lattice site \(A^{s_k}_k\), i.e. \(E = E(|A^{s_k}_k\rangle)\). The main task is to find the ground state wave function and its energy, that is, to find the global minimum of the function \(E(|A^{s_k}_k\rangle)\) and the corresponding value of \(A^{s_k}_k\).

This problem can be mapped to optimizing the total energy of a classical mechanical system, in which the elements of the tensor \(A^{s_k}_k\) are treated as the generalized coordinates of the system. We introduce the Lagrangian of the artificial system,

\[
\mathcal{L} = \frac{m}{2} \sum_{k=1}^N \sum_{s_k = 1}^d ||\dot{A}^{s_k}_k||^2 - E(|A^{s_k}_k\rangle), \tag{2}
\]

where \(m\) is the artificial mass of the ‘particles’, and we use\( m = 1\) in all the simulations. \(\dot{A}^{s_k}_k\) is the velocity of the corresponding matrix \(A^{s_k}_k\) defined on each lattice site. The norm of matrix \(||\dot{A}^{s_k}_k||\) is defined as

\[
||\dot{A}^{s_k}_k|| = \sqrt{\sum_{i,j=1}^D (\dot{a}^{s_k}_j(k))^2 (\dot{a}^{s_k}_i(k))}, \tag{3}
\]

where \(\dot{a}^{s_k}_j(k)\) is the velocity corresponding to \(a^{s_k}_j(k)\) which is the elements of \(A^{s_k}_k\).

We therefore have the Euler–Lagrange equation (we drop the site index \(k\) for simplicity),

\[
\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{a}^{s_k}_j} - \frac{\partial \mathcal{L}}{\partial a^{s_k}_j} = 0, \tag{4}
\]

which leads to,

\[
m \ddot{a}^{s_k}_j = -\frac{\partial E}{\partial a^{s_k}_j}. \tag{5}
\]

The energy and its derivative respect to given \(a^{s_k}_j\) can be easily calculated by MC sampling the physical configuration space [5, 9]. Since the MC sampling method for TNS has been described in details in [5, 9], we shall not repeat it here.

Equation (5) can be solved via the molecular dynamics (MD) method [19], using a velocity Verlet’s algorithm,

\[
\dot{a}^{s_k}_j(t + \Delta t) = \dot{a}^{s_k}_j(t) + \frac{1}{2} \Delta t [\ddot{a}^{s_k}_j(t) + \ddot{a}^{s_k}_j(t + \Delta t)], \tag{6}
\]

where,

\[
\ddot{a}^{s_k}_j(t + \Delta t) = \ddot{a}^{s_k}_j(t) + \frac{1}{2} \Delta t [\dddot{a}^{s_k}_j(t) + \dddot{a}^{s_k}_j(t + \Delta t)], \tag{7}
\]
and,

\[ m \tilde{a}_{ij}(t + \Delta t) = -\frac{\partial E}{\partial \tilde{a}_{ij}}(t). \]  

(8)

Now, we introduce a temperature \( T \) for each tensor \( A_k \) as the average ‘kinetic’ energies of the ‘particles’, i.e.

\[ T = \sum_i^D \sum_j^d \frac{|\tilde{a}_{ij}|^2}{N_D} \]  

(9)

where \( N_D = D^2d \) is the total degree freedoms (number of ‘particles’) of tensor \( A_k \). When the temperature approaches zero, both \( \tilde{a} \) and \( \dot{a} \) also approach zero, we then obtain the minimum of \( E((A_k^0)) \), i.e. the ground state energy of the quantum system, and corresponding wave function. When temperature \( T \) is sufficiently low, the system can be approximated as harmonic oscillations around their equilibrium positions, and therefore, according to the classical statistics the total energy of the system is \( E(T) \approx E_0 + D^2dT \).

We can run the MD simulation at a given temperature through exchanging energies with a heat bath. Since we are not interested in the real ‘dynamics’ of the system, one can use the simplest velocity rescaling thermostat. in order to fix the temperature at \( T \), we rescale the velocity \( \tilde{a}_{ij} \) by a factor \( \gamma = \sqrt{T/T^*} \) at each MD step, where \( T^* \) is the instantaneous temperature defined in equation (9). Note that when scaling a tensor \( A_k \), the energy of the system \( E((A_k^0)) \) remains unchanged. Therefore, we normalize the tensors by dividing them into the largest absolute value of the elements of each tensor after each MD step. Furthermore, any change in the tensor, \( A_k \), that is parallel to \( A_k \), during the MD steps has no contribution to the energy. To improve the efficiency, we orthogonalize the velocity \( \tilde{A}_k \) to \( A_k \) at each MD step before we rescaling the velocity to the given temperature,

\[ \tilde{A}_k = A_k - \frac{(A_k, A_k)}{(A_k, A_k)} A_k, \]  

(10)

where the inner product of two matrices is defined as,

\[ (A, B) = \sum_{i,j=1}^D A_{ij}^* B_{ij}. \]  

(11)

Usually the ground state energy of a simple system can be obtained by a simulated annealing method, i.e. one starts from a high temperature of the system, and gradually decreases the temperature to zero. If the temperature cooling is sufficiently slow, in principle one should get the global minimum of the system. However, since the energy is highly non-linear function of the tensors, and for frustrated physical models, which have many metastable states, in practice, it often easily trapped in some local minima.

Here, we adopt the replica exchange (also known as parallel tempering) \([12,13]\) MD method, which simulates \( M \) replicas simultaneously, and each at a different temperature \( \beta_0 = 1/T_{\text{max}} < \beta_1, \cdots, \beta_{M-2} < \beta_{M-1} = 1/T_{\text{min}} \) covering a range of interest, to avoid being stuck in local minima. Each replica runs independently, except after certain steps the configuration can be exchanged between neighboring temperatures, according to the Metropolis criterion,

\[ \omega = \frac{1}{e^{-\Delta H}} \]  

(12)

where \( \Delta H = -(\beta_1 - \beta_{i-1})(\bar{E}_i - \bar{E}_{i-1}) \) in which \( \bar{E}_i \) and \( \bar{E}_{i-1} \) are the average energies of the \( i \)-th and the \( (i - 1) \)-th replica in a range of certain MD steps. The inclusion of high-\( T \) configurations ensures that the lower temperature systems can access a broader phase space and avoid being trapped in local minima. During the simulation, we keep the highest temperature \( \beta_0 \) and lowest temperature \( \beta_{M-1} \) fixed, whereas the rest of the temperatures distribute exponentially between the highest and lowest temperatures at the start of simulation. During the simulation, the temperatures (except \( \beta_0 \) and \( \beta_{M-1} \)) are adjusted to ensure that the exchange rates between the replica are roughly equal \([16]\). Because the algorithm is intrinsically parallel in temperature, it is much more efficient than the traditional simulated annealing method.

The lower the minimal temperature \( T_{\text{min}} \), the more accurate the results one can obtain. In principle, \( T_{\text{min}} \) has to approach zero to get the real ground state. However, decreasing the \( T_{\text{min}} \) will increase the computational cost (the number of replica temperatures). Instead, one could continue to lower the temperature sequentially to a desired low temperature, or adopt a local energy minimizer (e.g. conjugate gradient method) after we finish the replica exchange MD simulations, to get more accurate ground state.

It is worth noting that a direct use of the Monte Carlo method instead of MD to update the tensors themselves (i.e. one directly changes the tensor elements according to the Metropolis criterion for the total energy) is not applicable for the scheme. The reason is that the energy obtained from MC sampling is not bounded from below. Therefore, it is very easy to be trapped in a false energy minimum (i.e. the energy minimum due to inadequate MC sampling, which may be much lower than the real energy of the system), especially if the sampling is not large enough, if a Monte Carlo updating method is used. In contrast, the MD method does not suffer from this problem.

3. Results and discussion

In this section, we present the benchmark tests of our scheme on the one-dimensional (1D) Hubbard model and two-dimensional (2D) \( J_1 - J_2 \) model. Since the 1D model has been well studied and has many efficient schemes, we simply present the results without detailed discussion. We discuss more detailed features of the scheme for the 2D model.

3.1. One-dimensional Hubbard model

To test our scheme, we compute the ground state energy of the 1D Hubbard model \([20]\),

\[ H = -\sum_{i} (c_{i\uparrow}^\dagger c_{i\downarrow} + \text{h.c.}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}. \]  

(13)
To simulate the 1D Hubbard model, we first transform it to a spin model via Jodran–Wigner transformation. The many-particle wave function of the ground state of the corresponding spin model via Jodran–Wigner transformation. The many-

To simulate the typical two dimensional frustrated spin-1/2 Heisenberg model, namely the j_1–j_2 model on a square lattice. The Hamiltonian of the model is,

\[ H = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j. \]  

The spin operators obey \( \mathbf{S}_i \cdot \mathbf{S}_j = S(S+1) = 3/4 \), whereas \( \langle i,j \rangle \) and \( \langle\langle i,j \rangle\rangle \) denote the nearest and next-nearest neighbor spin pairs, respectively, on the square lattice. j_1–j_2 model has become a promising candidate model whose ground state may be a spin liquid state near \( j_1/j_2 = 0.5 \) [21–23].

Two kinds of generalization to higher dimensions of MPS, i.e. PEPS and SBS can be used to simulate two dimensional systems. PEPS has extremely high scaling with the tensor dimension truncation \( D \), which are \( O(D^{12}) \), \( O(D^{18}) \) for OBC and PBC respectively [18]. In contrast, SBS has much lower scaling to \( D \), which are \( O(D^6) \) and \( O(D^3) \) for OBC and PBC respectively. Here, as a benchmark, we demonstrate our scheme using the SBS type of wave functions.
Figure 2. The evolution of the energies of the $J_1$–$J_2$ model with $J_2/J_1 = 0.7$ on a OBC lattice of size $6 \times 6$ during MD optimization. (a) The energy evolution at different temperatures as functions of the number of replica exchanges. (b) The energies as functions of temperature after 5, 30, 50, 150, 250 times of replica exchanges.

Figure 3. The ground state energies as functions of string patterns for the $J_1$–$J_2$ model on a $10 \times 10$ OBC lattice. S4 means that only the long string pattern is used with $D = 4$, whereas S8L4 means that both the long string pattern and loop pattern are used with $D = 8$ for the strings, and $D = 4$ for the loops.

Figure 4. Comparison of the ground state energies of the $J_1$–$J_2$ model on the OBC lattices of size (a) $4 \times 4$, (b) $6 \times 6$, and (c) $10 \times 10$. The black lines are the results obtained by the replica-MD method, whereas the red lines are the results taken from [18]. The PEPS results shown in blue lines for the $6 \times 6$, $10 \times 10$ lattices are also taken from [18].

Figure 5. The evolution of the energies of the $J_1$–$J_2$ model with $J_2/J_1 = 0.7$ on a OBC lattice of size $6 \times 6$ during MD optimization. (a) The energy evolution at different temperatures as functions of the number of replica exchanges. (b) The energies as functions of temperature after 5, 30, 50, 150, 250 times of replica exchanges.

The improvement of energy by increasing the virtual dimension cut-off $D$ and adding new SBS patterns are shown in figure 3 for a $10 \times 10$ OBC lattice, with $J_2 = 0, 0.5$ and 1.0. First, we use only the long strings. We find that $D = 8$ (S8) has converged the results. We then add the pattern of small loops, and the energies improve significantly. We find $D = 6$ (S8L6) for the loops converge the results. Further increase of the dimension $D$ for the loops does not improve the energy. As one can see that the energy obtained by SBS is still about 1–3% higher than the exact results or those obtained from PEPS. This error is from the limitation of the SBS wave functions, and is not from the optimization process [5, 18]. Unlike PEPS, the quality of SBS cannot be improved by simply increasing the dimension $D$ of the tensors alone. However, one can systematically improve the SBS by adding more patterns of the tensor strings [5]. Fortunately, the computational cost increases only linearly with the number of string patterns, in contrast to the extremely high scaling with the tensor dimension $D$ in the PEPS method. It is very valuable exchange, it may help the system from being stuck in some local minima.

Figure 2(b) depicts the total energies as functions of temperatures after 5, 30, 50, 150, 250 times of temperature exchanges for the above system. As we see that the energies at lower temperatures quickly decrease to near the ground state energy. After enough MD and temperature exchanges, the energy-temperature curves become stable. In this situation, we expect that we have obtained a good approximation to the ground state. We then further decrease the temperature to get a more accurate ground state energy.

The improvement of energy by increasing the virtual dimension cut-off $D$ and adding new SBS patterns are shown in figure 3 for a $10 \times 10$ OBC lattice, with $J_2 = 0, 0.5$ and 1.0. First, we use only the long strings. We find that $D = 8$ (S8) has converged the results. We then add the pattern of small loops, and the energies improve significantly. We find $D = 6$ (S8L6) for the loops converge the results. Further increase of the dimension $D$ for the loops does not improve the energy. As one can see that the energy obtained by SBS is still about 1–3% higher than the exact results or those obtained from PEPS. This error is from the limitation of the SBS wave functions, and is not from the optimization process [5, 18]. Unlike PEPS, the quality of SBS cannot be improved by simply increasing the dimension $D$ of the tensors alone. However, one can systematically improve the SBS by adding more patterns of the tensor strings [5]. Fortunately, the computational cost increases only linearly with the number of string patterns, in contrast to the extremely high scaling with the tensor dimension $D$ in the PEPS method. It is very valuable.
to study how to improve the SBS wave functions by adding new types of string patterns. We leave this for future study.

We then compare the obtained results using the method described in this paper with the results obtained from the exact diagonalization method or PEPS method, and those in [18] which also used SBS on lattices of size 4 × 4, 6 × 6 and 10 × 10 with both OBC and PBC in figure 4 and figure 5, respectively. It can be seen that for the OBC, the ground state energies optimized by the replica-MD method are significantly improved from the ones obtained using the original optimization method. In the case of PBC, the ground state energies are also better than those obtained in [18], although less significant.

It is worth pointing out that the MD optimization scheme developed in this work can apply not only to the MPS and SBS types of TNS, but also to general TNS, e.g. PEPS with some modification [10]. It is suitable to study the systems with a rough energy surface, where other optimization methods may fail. The current method with MC sampling has other advantages, e.g. it is easy to implement the constraints in physical space. For example, it is easy to simulate the system in a canonical ensemble using this method, with particle number conservation, as well as the grand canonical ensemble with fixed chemical potential, whereas it is difficult to enforce particle number conservation in the contraction methods.

4. Summary

The tensor network states method has been proved a powerful algorithm for simulating quantum many-body systems. However, because the ground state energy is a highly non-linear function of the tensors, it is easy to be trapped in the local minima when optimizing the TNS of the simulated physical systems. We have introduced a replica exchange molecular dynamics method to optimize the tensor network states. We demonstrate the method on a one dimensional Hubbard model based on MPS and the two dimensional frustrated Heisenberg J1−J2 model on square lattices based on SBS. For the one dimensional model, our results are in excellent agreement with those from the exact diagonalization method. For the two dimensional model, our results show an improvement over the existing calculations, especially in the strong frustrated region. The method can be generalized to other forms of TNS, e.g. PEPS with some modification, and provides a useful tool to investigate complicated many-particle systems, such as frustrated systems and fermionic systems.

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References

[1] Vidal G 2003 Phys. Rev. Lett. 91 147902
[2] Vidal G 2004 Efficient simulation of one-dimensional quantum many-body systems Phys. Rev. Lett. 93 040502
[3] Fannes M, Nachtergaele B and Werner R F 1992 Finitely correlated states on quantum spin chains Commun. Math. Phys. 144 443–90
[4] Verstraete F and Cirac J I 2004 Renormalization algorithms for quantum-many body systems in two and higher dimensions (arXiv:cond-mat/0407056)
[5] Schuch N, Wolf M M, Verstraete F and Cirac J I 2008 Simulation of quantum many-body systems with strings of operators and Monte Carlo tensor contractions Phys. Rev. Lett. 100 040501
[6] Vidal G 2007 Entanglement renormalization Phys. Rev. Lett. 99 220405
[7] Verstraete F, Porras D and Cirac J I 2004 Density matrix renormalization group and periodic boundary conditions: a quantum information perspective Phys. Rev. Lett. 93 227205
[8] Murg V, Verstraete F and Cirac J I 2007 Variational study of hard-core bosons in a 2D optical lattice using projected entangled pair states Phys. Rev. A 75 033605
[9] Sandvik A W and Vidal G 2007 Variational quantum Monte Carlo simulations with tensor-network states Phys. Rev. Lett. 99 220602
[10] Wang L, Pizorn I and Verstraete F 2011 Monte Carlo simulation with tensor network states Phys. Rev. B 83 134421
[11] Waldtmann C, Everts H-U, Bernu B, Lhuillier C, Sindzingre P, Lecheminant P and Pierre L 1998 First excitations of the spin-1/2 Heisenberg antiferromagnet on the Kagomé lattice Eur. Phys. J. B 2 501
[12] Swendsen R H and Wang J-S 1986 Replica Monte Carlo simulation of spin-glasses Phys. Rev. Lett. 57 2607–9
[13] Geyer C J 1991 Computer Science and Statistics Proc. of the 23rd Symp. on the Interface (Seattle, WA, 21–24 April 1991) (Fairfax Station, VA: Interface Foundation)
[14] Marinari E, Parisi G and Ruiz-Lorenzo J J 1998 Phys. Rev. B 58 14852
[15] Cao K, Guo G-C, Vanderbilt D and He L 2009 Phys. Rev. Lett. 103 257201
[16] Cao K, Zhou Z-W, Guo G-C and He L 2010 Efficient numerical method to calculate the three-tangle of mixed states Phys. Rev. A 81 034302
[17] Fisher M P A, Weichman P B, Grinstein G and Fisher D S 1989 Boson localization and the superfluid-insulator transition Phys. Rev. B 40 546–70
[18] Sfondrini A, Cerrillo J, Schuch N and Cirac J I 2010 Simulating two- and three-dimensional frustrated quantum systems with string-bond states Phys. Rev. B 81 244426
[19] Haile J M 1997 Molecular Dynamics Simulation: Elementary Methods (New York: Wiley)
[20] Frahm H, Göhmann F, Klümpner A and Korepin V E 2005 The One-Dimensional Hubbard Model (Cambridge: Cambridge University Press)
[21] Wang L, Gu Z-C, Verstraete F and Wen X-G 2012 Spin-liquid phase in spin-1/2 square $j_1$–$j_2$ heisenberg model: a tensor product state approach (arXiv:1112.3331)
[22] Wang L, Poilblanc D, Gu Z-C, Wen X-G and Verstraete F 2013 Phys. Rev. Lett. 111 037202
[23] Jiang H-C, Yao H and Balents L 2012 Phys. Rev. B 86 024424
[24] Wang Z, Han Y, Guo G-C and He L 2013 Size consistency of tensor network methods for quantum many-body systems Phys. Rev. B 88 121105
[25] Schulz H J, Ziman T A L and Poilblanc D 1996 Magnetic order and disorder in the frustrated quantum heisenberg antiferromagnet in 2D J. Phys. I 6 675