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Numerical study of spin-1/2 XXZ model on square lattice from tensor product states

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Abstract. By means of the recently proposed algorithm based on the tensor product states, the magnetization process of the spin-1/2 antiferromagnetic XXZ model on a square lattice is investigated. In the large spin-anisotropy limit, clear evidence of a first-order spin–flip transition is observed as an external magnetic field is increased. Our findings of the critical field and the discrete jumps in various local order parameters are in good agreement with the quantum Monte Carlo data in the literature. Our results imply that this algorithm can be an accurate and efficient numerical approach in studying first-order quantum phase transitions in two dimensions.

Keywords: other numerical approaches, quantum phase transitions (theory), renormalization group

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Contents

1. Introduction

Numerical simulations are usually required in the theoretical investigation of strongly correlated systems, because analytical solutions are not available in most cases. Consequently, developing accurate and efficient numerical tools becomes one of the central issues in the understanding of quantum many-body systems. Recently, based on an efficient representation of a two-dimensional system's wavefunction through a tensor network, a series of new simulation algorithms has been achieved. In particular, the infinite projected entangled-pair states (iPEPS) algorithm [1] has been proposed and applied to various interesting systems with success [2]–[6]. In this approach, the ground-state wavefunction is described by the so-called tensor product state (TPS) [7, 8] or the projected entangled-pair state (PEPS) [9, 10]. Taking into account possible translational symmetry in the ground state, such a tensor network can be simply represented by copies of a small number of tensors even for systems on infinite lattices. After optimizing these tensors under specific prescriptions, a number of physical properties can be calculated from the optimized TPS/PEPS.

By handling tensor product wavefunctions in different manners, schemes distinct from the iPEPS algorithm have also been put forward [11, 12]. A virtue of these approaches is that they can be implemented with ease. In [11], the optimized TPSs are determined via direct variational approach, where the variational energies of systems of very large sizes are efficiently evaluated by means of the tensor renormalization group (TRG) method [13, 14]. The expectation values of physical quantities are then calculated from the optimized TPS, again under the TRG method. This algorithm has been tested for several two-dimensional (2D) quantum spin models [11] and the results agree well with previous findings. Alternatively in [12], the ground states of a TPS form are obtained by using the power method through iterative projections. This approach can be considered as a generalization of the 1D infinite time-evolving block decimation (iTEBD) method [15] to the two-dimensional cases. After getting the ground states, the TRG method [13] is employed to calculate the expectation values of physical observables. It is shown that accurate results for the Heisenberg model on a honeycomb lattice can be reached under this approach [12].

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Due to the simplicity and efficiency of the iTEBD and the TRG algorithms, the approach proposed in [12] can become one of the most promising numerical methods in studying quantum many-body systems once its general validity is established. Recently, it is shown that the TPS/PEPS ansatz is suited to study the first-order phase transition [3]. However, because of the difference in optimizing ground states and in evaluating expectation values, one may wonder if the combined iTEBD and TRG algorithm can determine the first-order phase transitions to the same accuracy as the iPEPS algorithm does.

In order to provide a further benchmark on the performance of the combined iTEBD and TRG algorithm, in this work we investigate the magnetization process of the spin-1/2 antiferromagnetic XXZ model on a square lattice. Here the large spin-anisotropy case is considered, where the existence of first-order spin-flip transitions in the magnetization process has been established by means of quantum Monte Carlo (QMC) simulations [16, 17][3]. We find that various local order parameters defined below change discontinuously at a critical field, which clearly indicates the appearance of a first-order transition. Moreover, satisfactory results of the critical field and the discrete jumps in the local order parameters are obtained as compared to the previous QMC findings [17]. Our present investigation suggests that this combined algorithm should also be an effective numerical method in studying first-order quantum phase transitions in two dimensions.

2. Tensor network algorithm

Before presenting our results, it is instructive to sketch the combined iTEBD and TRG algorithm employed here. We know that the ground state can, in principle, be determined through the imaginary time evolution for a given initial state $|\Psi_0\rangle$: $|\Psi_{\rm GS}\rangle = \lim_{\tau\to\infty} \exp(-H\tau)|\Psi_0\rangle/\|\exp(-H\tau)|\Psi_0\rangle\|$. If, just like the present case, the model Hamiltonian can be written as a sum of terms $h_{\langle i,j\rangle}$ involving only pairs of nearest-neighboring sites i and j, the Suzuki–Trotter formula [19] can be exploited to decompose the imaginary time evolution operation into a product of two-site evolution operators: $U_{\langle i,j\rangle} = \exp(-h_{\langle i,j\rangle}\delta\tau)$, where $\delta\tau \ll 1$. It is also known that any wavefunction can always be approximated in a TPS form. A possible construction of TPS for systems on a square lattice is to attach a rank-five tensor $[\Gamma_i]^s_{lrud}$ to each site i and a diagonal singular value matrix (hence a vector) $[\lambda_{\langle i,j\rangle}]_l$ to each bond of nearest-neighboring sites i and j. Here s is the physical index with $s = 1, 2$ for the present spin-1/2 case and l, r, u, d $(=1\cdots D)$ denote the virtual bond indices in four directions. In general, better representation of a given wavefunction can be achieved by increasing the bond dimension D. Taking into account the possible translational symmetry in the ground state under shifts by two lattice sites both in the x and y directions, the tensor network can be simply represented by copies of tensors within a 2×2 unit cell. That is, we are left with four independent Γ_i tensors and eight independent $\lambda_{\langle i,j\rangle}$ matrices. The action of a two-site evolution operator $U_{\langle i,j\rangle}$ on such a TPS can be absorbed by performing a singular value decomposition, and thus leads to an update of the Γ_i, Γ_j, and $\lambda_{\langle ij\rangle}$ tensors [12]. When eight nearest-neighboring bonds within the 2×2 unit cell are all updated, a complete iteration is achieved. After

[3] It is known that the Hamiltonian in equation (3) is equivalent to a hard-core boson model under the mapping: $a_j^\dagger = S_j^x + iS_j^y$, $a_j = S_j^x - iS_j^y$ and $n_j = a_j^\dagger a_j = (S_j^z + 1/2)$, where $a_j^\dagger$ is a creation operator of a hard-core boson at site j. Thus the same results are also found in terms of the boson language. For example, see [18].

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a sufficient time of such updating iterations, the optimized ground state of the TPS form can be generated.

Since evaluation of the expectation values for a TPS under the most straightforward method is exponentially difficult, for a complete numerical algorithm, an efficient way to do these calculations for large systems must also be constructed. Here the TRG approach [11, 13] is employed. For any operator that can be decomposed into a product of local operators, $\hat{O} = \prod_i \hat{O}_i$, evaluating $\langle \Psi_{\mathrm{GS}} | \hat{O} | \Psi_{\mathrm{GS}} \rangle$ for the TPS ground state $|\Psi_{\mathrm{GS}}\rangle$ is equivalent to compute the contraction of a corresponding tensor network of $\mathbf{T}$ tensors. Within such a tensor network, the rank-four tensor $\mathbf{T}^i$ at site i is defined as

$$[\mathbf{T}^i]_{\bar{l}\bar{r}\bar{u}\bar{d}} = \sum_{ss'} \langle s' | \hat{O}_i | s \rangle [A^i]^s_{lrud} ([A^i]^{s'}_{l'r'u'd'})^* \tag{1}$$

with

$$[A^i]^s_{lrud} \equiv \sqrt{[\lambda_{\langle i,i-\hat{x}\rangle}]_l [\lambda_{\langle i,i+\hat{x}\rangle}]_r [\lambda_{\langle i,i+\hat{y}\rangle}]_{\mathrm{u}} [\lambda_{\langle i,i-\hat{y}\rangle}]_d} [\Gamma_i]^s_{lrud}, \tag{2}$$

where $|s\rangle$ represents the spin state at site i. $i \pm \hat{x}$ and $i \pm \hat{y}$ denote the nearest neighbors of site i in the x and y directions, respectively. $\bar{l} = (l, l')$ is the double bond index and $\bar{r}, \bar{u}, \bar{d}$ are similarly defined. The tensor network of $\mathbf{T}$ tensors can then be coarse-grained in an iterative fashion [11, 13]. Each complete renormalization group (RG) step reduces the size of the network by a factor of two. The accuracy of such an RG process is controlled by a cutoff D_{cut} on the double bond indices of the coarse-grained tensor. Therefore, to evaluate the contraction of the tensor network of size $2^{n+1} \times 2^{n+1}$, we need only perform n RG steps. To sum up, the TPS provides an efficient way to approximate the 2D wavefunctions. The agreement between the actual wavefunction and the represented TPS wavefunction can be improved simply by increasing the bond dimension D. Besides, the TRG approach serves as an efficient tool to evaluate the expectation values for a TPS ground state of very large systems, where the accuracy can be systematically improved by increasing the cutoff D_{cut}. In the present work we consider the bond dimension up to $D = 5$ and keep $D_{\mathrm{cut}} \geq D^2$ to ensure the accuracy of the TRG calculation.

The general simulation procedure is described as follows. For a given h and D, we take a set of random Γ and λ tensors as our initial state $|\Psi_0\rangle$. While the initial state may not have the spatial rotational symmetry, during the imaginary time evolution, the evolved state will converge towards a ground state which respects this expected symmetry. It hence provides a self-consistent stability check for the algorithm. To minimize the Trotter error, we usually start with $\delta\tau = 10^{-1}$ and gradually decrease it to $\delta\tau = 10^{-3}$ to ensure the convergence of the wavefunction.

3. Results

In the following, we present our numerical results for the spin-1/2 XXZ model with system size $N = 2^7 \times 2^7$. In the presence of an external magnetic field h along the z direction,

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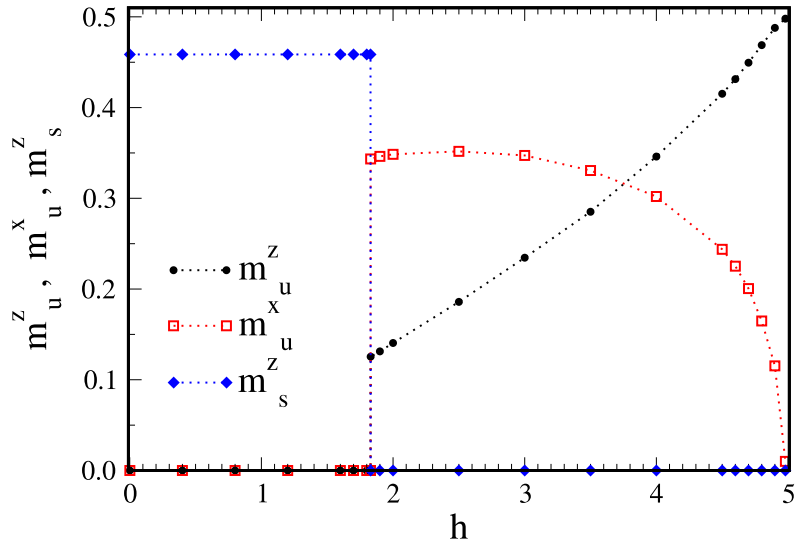

Figure 1. Values of $m^z_{\rm u}$, $m^x_{\rm u}$ and $m^z_{\rm s}$ for the ground state at $\Delta = 1.5$ as functions of external field h for systems of size $2^7 \times 2^7$ with $D = 4$ and $D_{\rm cut} = 16$.

the Hamiltonian of the XXZ model is given by[4]

$$H = J\sum_{\langle i,j\rangle}(-S^x_i S^x_j - S^y_i S^y_j + \Delta S^z_i S^z_j) - h\sum_i S^z_i, \tag{3}$$

where S^α_i is the α $(=x, y, z)$ component of the spin-1/2 operator at site i and $\langle ij\rangle$ runs over all the nearest-neighboring pairs of spins at sites i and j. $J \equiv 1$ is the exchange coupling and Δ (≥ 0) is an anisotropic parameter. We focus our attention on the large spin-anisotropy case of $\Delta = 1.5$, where accurate QMC calculations have been performed [17]. The expectation values of the z-component staggered magnetization $m^z_{\rm s} \equiv \sum_i \langle S^z_i\rangle {\rm e}^{{\rm i}\mathbf{Q}\cdot\mathbf{r}_i}/4$, the uniform one $m^z_{\rm u} \equiv \sum_i \langle S^z_i\rangle/4$ and the x-component uniform magnetization $m^x_{\rm u} \equiv \sum_i \langle S^x_i\rangle/4$ for the ground states $|\Psi_{\rm GS}(h)\rangle$ are shown in figure 1, where $\mathbf{Q} = (\pi, \pi)$ and the sum on i runs over four sites within the 2×2 unit cell under consideration. Here we take the bond dimension $D = 4$ and the TRG cutoff $D_{\rm cut} = 16$. We note that results for $D = 3, 5$ are very similar to those for $D = 4$ and are thus not shown here. In the large spin-anisotropy limit with $\Delta > 1$, it is known that a first-order spin–flip transition from a Néel-ordered phase to a spin-flopping phase will occur as the external field h increases from zero [16, 17] (see footnote 3). Crossing the critical field $h_{\rm c}$, the z-component staggered magnetization $m^z_{\rm s}$ suddenly drops to zero and the uniform part $m^z_{\rm u}$ jumps to a nonzero value. When $h > h_{\rm c}$, $m^z_{\rm u}$ increases monotonically and finally reaches its saturated value $(m^z_{\rm u} = 1/2)$ at $h = h_{\rm s}(=2(1+\Delta))$, while the staggered one $m^z_{\rm s}$ remains zero. A character of the spin-flopping states for $h_{\rm c} < h < h_{\rm s}$ is the existence of finite x-component magnetization $m^x_{\rm u}$, whose value gives a measure of spin superfluidity (see below). When spins become fully polarized in the z direction as h approaches $h_{\rm s}$, $m^x_{\rm u}$

[4] The Hamiltonian described in equation (3) is equivalent to that of the conventional antiferromagnetic XXZ model by the following unitary transformation: rotating the spins along the z axis with an angle π (thus $S^x_i \to -S^x_i$ and $S^y_i \to -S^y_i$) on the sublattice consisting of, say, even sites.

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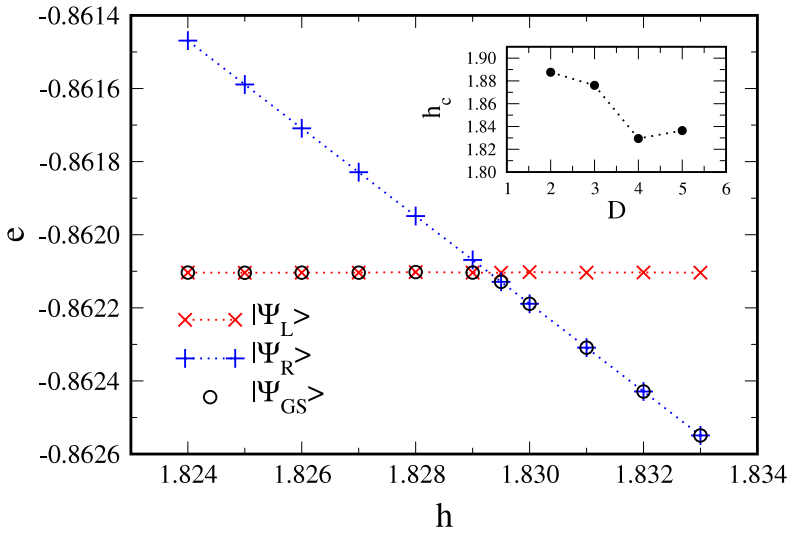

Figure 2. Energies $e(h)$ per site for the adiabatically evolved states $|\Psi_{\rm L}(h)\rangle$ and $|\Psi_{\rm R}(h)\rangle$. The values for the ground state $|\Psi_{\rm GS}(h)\rangle$ are denoted by open circles. Here $\Delta = 1.5$ for systems of size $2^7 \times 2^7$ with $D = 4$ and $D_{\rm cut} = 16$. The inset shows the critical field $h_{\rm c}$ for various D ($D_{\rm cut} = 16$ for $D \leq 4$ and $D_{\rm cut} = 25$ for $D = 5$). The dotted line is a guide to the eyes.

will decrease to zero. As seen from figure 1, our values of $m_{\rm s}^z$, $m_{\rm u}^z$ and $m_{\rm u}^x$ do show the expected results.

Typically a first-order quantum phase transition comes from energy level crossing in the ground state and the crossing point gives the critical value of the tuning parameter [20]. In the present case, the relevant states should be the ground state in the Néel-ordered phase with zero $m_{\rm u}^z$ and that in the spin-flopping phase with finite $m_{\rm u}^z$. Here we simulate the adiabatically evolved states $|\Psi_{\rm L}(h)\rangle$ and $|\Psi_{\rm R}(h)\rangle$ starting from the computed ground states in the Néel-ordered phase and in the spin-flopping phase, respectively. That is, $|\Psi_{\rm L}(h)\rangle$ ($|\Psi_{\rm R}(h)\rangle$) are determined starting from the ground state $|\Psi_{\rm GS}(h_{\rm ini})\rangle$ for a given initial parameter $h_{\rm ini} < h_{\rm c}$ ($h_{\rm ini} > h_{\rm c}$) and adiabatically increasing (decreasing) h in the Hamiltonian well beyond crossing the critical field $h_{\rm c}$. True ground states $|\Psi_{\rm GS}(h)\rangle$ are the ones with lower energies. The corresponding energies $e(h)$ per site are shown in figure 2 for $D = 4$ and $D_{\rm cut} = 16$. We find that the energies of $|\Psi_{\rm L}(h)\rangle$ remain unchanged as h varies, while those of $|\Psi_{\rm R}(h)\rangle$ are lowered as h increases. This is expected since $|\Psi_{\rm L}(h)\rangle$ should behave like Néel-ordered states with zero $m_{\rm u}^z$ and thus their energies do not depend on the external field. However, $|\Psi_{\rm R}(h)\rangle$ should retain the spin-flopping character with nonzero $m_{\rm u}^z$, hence their energy expectation value $\langle H\rangle$ for the Hamiltonian in equation (3) should behave as a decreasing function of h. Due to level crossing in these two states, discontinuity in the first derivative of the ground-state energy appears. This again indicates the presence of a first-order quantum phase transitions. From the crossing point in figure 2, we find that $h_{\rm c} \sim 1.829$, which is quite close to the value estimated by QMC ($h_{\rm c} \sim 1.83$) [17]. The dependence of $h_{\rm c}$ on the bond dimension D is plotted in the inset of figure 2. While the findings of $h_{\rm c}$ for $D = 2$ and 3 are somewhat higher than the QMC result, satisfactory values can be obtained for larger D.

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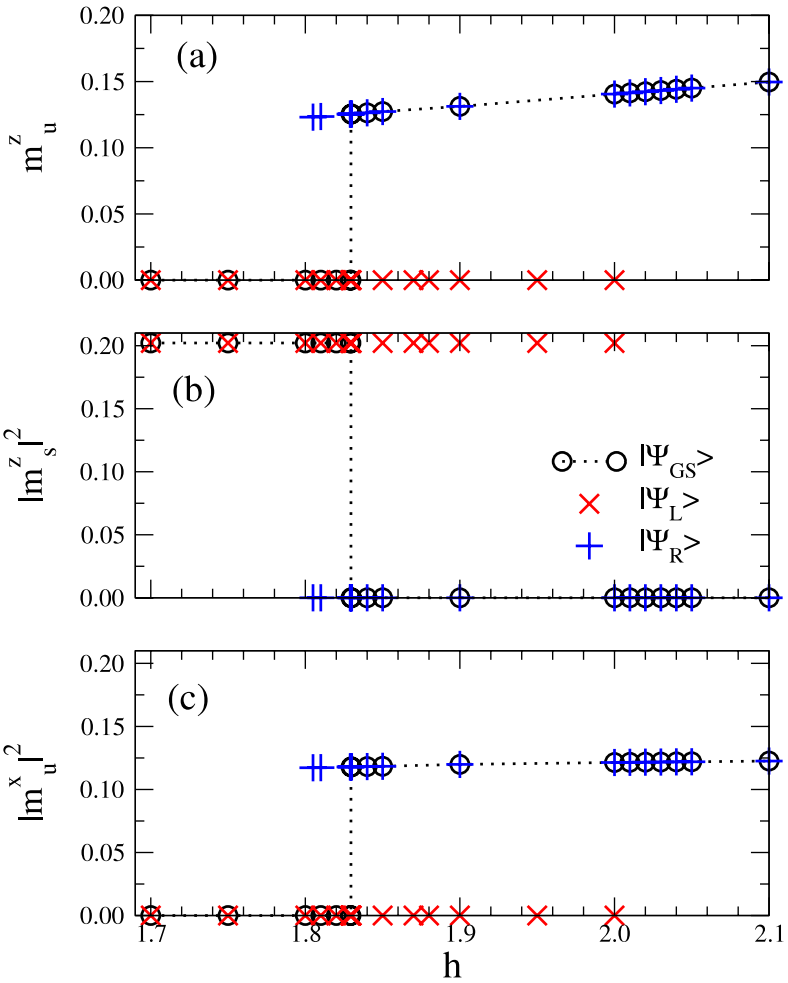

Figure 3. Values of (a) $m^z_{\rm u}$, (b) $|m^z_{\rm s}|^2$ and (c) $|m^x_{\rm u}|^2$ for the adiabatically evolved states $|\Psi_{\rm L}(h)\rangle$ and $|\Psi_{\rm R}(h)\rangle$. The values for the ground state $|\Psi_{\rm GS}(h)\rangle$ are denoted by open circles. Here $\Delta = 1.5$ for systems of size $2^7\times 2^7$ with $D = 4$ and $D_{\rm cut} = 16$.

To show further evidence of a first-order transition between the Néel-ordered phase and the spin-flopping phase, the results of $m^z_{\rm u}$, $|m^z_{\rm s}|^2$ and $|m^x_{\rm u}|^2$ for the adiabatically evolved states $|\Psi_{\rm L}(h)\rangle$ and $|\Psi_{\rm R}(h)\rangle$, and the corresponding values for the ground state $|\Psi_{\rm GS}(h)\rangle$ are displayed in figure 3. We find that the values of $m^z_{\rm u}$, $|m^z_{\rm s}|^2$ and $|m^x_{\rm u}|^2$ for the ground state are all discontinuous at $h_{\rm c}$. Moreover, all the results for the adiabatically evolved states $|\Psi_{\rm L}(h)\rangle$ and $|\Psi_{\rm R}(h)\rangle$ show clearly the hysteresis behavior. These facts strongly support the presence of a first-order transition. The discrete jumps at $h_{\rm c}$ for $m^z_{\rm u}$ and $|m^z_{\rm s}|^2$ are $m^z_{\rm u,c} \sim 0.125$ and $|m^z_{\rm s,c}|^2 \sim 0.202$, respectively. Both of them agree with the QMC results reported in [17]: $m^z_{\rm u,c} \sim 0.11$ and $|m^z_{\rm s,c}|^2 \sim 0.20$[5]. As mentioned before, in the spin-flopping phase for $h_{\rm c} < h < h_{\rm s}$, there exists spin superfluidity which can be characterized by nonzero spin stiffness $\rho_{\rm s}$ (or the superfluid density in the corresponding

[5] Within the Néel-ordered phase, one can show that $S(\mathbf{Q})/N = |m^z_{\rm s}|^2$ in the thermodynamic limit, where $S(\mathbf{Q}) \equiv (1/N)\sum_{i,j}\langle \mathbf{S}_i \cdot \mathbf{S}_j\rangle e^{i\mathbf{Q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}$ is the spin structure factor. The QMC data for $S(\mathbf{Q})/N$ in the thermodynamic limit can be read off from figure 2(b) of [17].

hard-core boson model). It is shown that ρ_s changes discontinuously at the first-order spin-flip transition [17]. To the best of our knowledge there is no straightforward way to calculate the spin stiffness ρ_s within the TPS framework. Instead, the square of the x-component magnetization m_u^x is evaluated, which can be related to the density of the Bose condensate in the corresponding hard-core boson model[6]. Thus the fact of non-vanishing $|m_u^x|^2$ also implies the existence of spin superfluidity. As seen from figure 3(c), similar to the behavior of ρ_s observed in the QMC study, $|m_u^x|^2$ has also a discrete jump at h_c, which is of magnitude $|m_{u,c}^x|^2 = 0.118$.

4. Conclusion

In summary, the first-order spin-flip transition of the spin-1/2 XXZ model with large spin anisotropy can be detected under the combined iTEBD and TRG algorithm proposed in [12]. Good agreement with the accurate QMC calculations can be obtained by using merely moderate bond dimension D and the TRG cutoff D_{cut}. This demonstrates that the current formalism will be a competitive numerical method to determine particularly a first-order quantum phase transition in two dimensions, with simplicity and efficiency as its advantages. We note, however, that further investigations are necessary to establish its general validity and to explore its relative performance as compared to other TPS/PEPS-based approaches.

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[6] For the spin-flopping states with the in-plane magnetization along the x direction, by using the relations between boson operators and the spin ones (see footnote 3), we have $\rho_0 = |m_u^x|^2$ in the thermodynamic limit. Here ρ_0 is the Bose condensate fraction in the hard-core boson model given by $\rho_0 = (1/N^2)\sum_{i,j}\langle a_i^\dagger a_j\rangle$.

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