Quantum Monte Carlo Study of Random Antiferromagnetic Heisenberg Chain

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Abstract. Effects of randomness on the spin-$\frac{1}{2}$ and 1 antiferromagnetic Heisenberg chains are studied using the quantum Monte Carlo method with the continuous-time loop algorithm. We precisely calculated the uniform susceptibility, string order parameter, spatial and temporal correlation length, and the dynamical exponent, and obtained a phase diagram. The generalization of the continuous-time loop algorithm for the systems with higher-$S$ spins is also presented.

1. Introduction

Low-energy properties of one-dimensional quantum Heisenberg antiferromagnets have been of great interest for many years. Particularly, effects of randomness on ground states with strong quantum fluctuations, such as the so-called Haldane state, have been studied extensively in recent years [1-5].

In the present work, we investigated $S = \frac{1}{2}$ and $S = 1$ random antiferromagnetic Heisenberg chains by means of the quantum Monte Carlo method with the continuous-time loop algorithm [6-9]. To this end, we first generalize this algorithm to systems with $S = 1$ or higher. This quite powerful simulation technique enables us precise calculations of thermodynamic quantities, such as the uniform susceptibility, etc.

2. Model and Numerical Method

We consider the spin-$S$ antiferromagnetic Heisenberg chain of $L$ spins with random nearest-neighbor interaction:

$$\mathcal{H} = \sum_{i=1}^{L} J_i (\mathbf{S}_i \cdot \mathbf{S}_{i+1}) ,$$

where $\mathbf{S}_i$ is a spin operator at site $i$ and $\mathbf{S}_i^2 = S(S+1)$. A periodic boundary condition is applied. All of $J_i$'s are taken to be positive (antiferromagnetic).

It is well known that traditional world-line Monte Carlo methods [6] suffer from long auto-correlation time at low temperatures. This difficulty is solved by the loop algorithm [7,8]. In addition, one can completely eliminate the systematic error beforehand, which is due to the discreteness in the imaginary-time

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direction, by adopting the recently proposed continuous-time algorithm [9]. The continuous-time loop algorithm, which was originally proposed for a spin-\( \frac{1}{2} \) system, can be generalized in a straightforward way to the spin-1 or higher systems as shown below [10].

First, we introduce spin-\( \frac{1}{2} \) representations of the partition function of the Hamiltonian (1):

\[
Z = \sum_{\{n\}} \langle n | \exp[-\beta \tilde{\mathcal{H}}]P | n \rangle, \tag{2}
\]

where

\[
\tilde{\mathcal{H}} = \sum_{i=1}^{L} \sum_{\mu,\nu=1}^{2S} \frac{J_{i}}{4} (\sigma_{i,\mu} \cdot \sigma_{i+1,\nu}). \tag{3}
\]

Each \( S_i \) is now represented as a sum of \( 2S \) Pauli operators (\( \sigma_{i,1}, \sigma_{i,2}, \cdots, \sigma_{i,2S} \)) and the trace in Eq. (2) is taken over the complete basis \( \{n\} \) of the space spanned by the \( 2SL \) Pauli operators. The projection operator \( P = \prod_{i} P_{i} \) projects out unphysical states, which do not appear in the original phase space of dimension \((2S+1)^L\). After performing the Suzuki-Trotter decomposition, we obtained the partition function of the (1+1)-dimensional classical Ising model with four-body weights of \( \exp[-\beta J_{i} \sigma_{i,\mu} \sigma_{i+1,\nu}/4m] \) and additional \((4S)\)-body weights of \( P_i \) at the boundaries in the imaginary-time direction.

Note that each four-body weight is completely equivalent to that appears in the world-line representation of the spin-\( \frac{1}{2} \) system. Therefore, in constructing a loop algorithm, assignment probabilities of graphs for these weights remain unchanged. For a boundary \((4S)\)-body weight, we consider \((2S)!\) types of graphs, each of which consists of \( 2S \) edges connecting one of \( \frac{1}{2} \) spins at \( \tau = \beta \) with a \( \frac{1}{2} \) spin at \( \tau = 0 \) one by one. A graph is called ‘compatible,’ if every pair of spins connected by an edge have a same direction. A graph is selected out of such compatible graphs with equal probability. After the assignment procedure, loops are identified to be flipped independently with probability \( \frac{1}{2} \).

The continuous-time limit (so-called Trotter limit) of the above procedure clearly exists. This is the most significant advantage of the present algorithm when one makes a comparison with the discrete version of the general-S loop algorithm, proposed by Kawashima and Gubernatis [12]. The present method also works with the XXZ model, systems in higher dimensions, and even systems with mixed magnitude of spins without any changes on the algorithm.

We have calculated the spin-spin correlation function of the clean antiferromagnetic Heisenberg chain with \( S = \frac{1}{2}, 1, \cdots, \frac{5}{2} \). The correlation length in the zero temperature limit is estimated as \( \xi \simeq 6.02 \) and 49.6 for \( S = 1 \) and 2 cases, respectively, while we observed power-law divergence with the inverse temperature in the cases with half-integer spins. The estimates for \( S = 1 \) and 2 agree quite well with the recent results by the density matrix renormalization group method [13,14].
3. Results

We consider the uniformly-distributed bond randomness with dimerization:

\[ J_i = 1 + (-1)^i u + \delta_i \]

with

\[ P(\delta_i) = \begin{cases} 1/W & \text{for } -W/2 < \delta_i < W/2 \\ 0 & \text{otherwise} \end{cases} \]

The parameters \( W \) and \( u \) control the strength of the randomness and the dimerization, respectively. For \( |u| + W/2 \leq 1 \), all \( J_i \)'s are antiferromagnetic.

3.1. \( S = \frac{1}{2} \) random Heisenberg chain

The clean (i.e. \( W = 0 \) and \( u = 0 \)) \( S = \frac{1}{2} \) antiferromagnetic Heisenberg chain has no excitation gap. By introduction of infinitesimal randomness, the system is driven to the random singlet (RS) phase. In this phase, it is shown that there is also no excitation gap, but the antiferromagnetic correlation of spins decays with a different exponent from that in the clean case [1,2].

In Fig. 1, we show the uniform susceptibility in the cases with \((W, u) = (1,0)\) and \((2,0)\). The random average was taken over 3000 samples for the lowest temperature \((T = 0.001)\) in the calculation. The uniform susceptibility diverges as the temperature goes down, which makes a sharp contrast with the clean \((W = 0)\) case. As seen in Fig. 1, \((\chi T)^{-1/2}\) plotted versus \(\log T\) lies on a straight line at low temperatures in both cases. This implies the uniform susceptibility behaves as \(\chi \sim 1/T(\log T)^2\), which is consistent with the prediction of the real-space renormalization group (RSRG) theory [2].

Figure 1: Uniform susceptibility in the RS phase of the \( S = \frac{1}{2} \) random antiferromagnetic Heisenberg chain with bond distribution \((W, u) = (1,0)\) and \((2,0)\).
Figure 2: Exponent $\gamma$, spin gap $\Delta$, and square root of the inverse spatial correlation length $\xi^{-1/2}$ of the $S = \frac{1}{2}$ dimerized random antiferromagnetic Heisenberg chain with $u + \frac{W}{2} = 1$.

3.2. $S = \frac{1}{2}$ random chain with dimerization

If a weak dimerization $u$ is enforced with $u + \frac{W}{2}$ fixed to 1, the spin correlation becomes short ranged immediately, while the spin gap remains closed until $u \simeq 0.27$ (Fig. 2). This phase is referred to as the random dimer (RD) phase, and a realization of the quantum Griffiths phase [2,3]. In the RD phase, the exponent $\gamma$ of the uniform susceptibility ($\chi \sim T^{-\gamma}$) varies continuously and diverges to the negative infinity at the end of the RD phase.

The string order parameter $O_{str}$ exists in the dimer phase and also in the RD phase. We found near the RS point ($u = 0$), $O_{str}$ is well scaled by a logarithmic scaling form:

$$O_{str} \sim L^{-2\beta/\nu} f(u L^{1/\nu}, L^{1/\nu} / \log T)$$

with $\nu = 2$ and $\beta = 0.382$ as predicted by the RSRG arguments [2,3]. This implies the dynamical exponent $z$ is actually infinite in the RS phase.

3.3. $S = 1$ random Heisenberg chain

Finally, we consider the $S = 1$ chain without dimerization. We found almost similar behavior of the uniform susceptibility as in the case of the $S = \frac{1}{2}$ dimerized case discussed above. For small randomness $W$, the system has the so-called Haldane gap. As the strength of the randomness increases, the exponential behavior of the susceptibility changes to the power-law behavior at $W \sim 1.5$.

For the extremely wide bond distribution ($W = 2$), we have confirmed that the uniform susceptibility obeys the same asymptotic form $\chi \sim 1/T(\log T)^2$ as in the RS phase of the $S = \frac{1}{2}$ case.
4. Summary and Discussions

Results of the precise quantum Monte Carlo simulation of the random antiferromagnetic Heisenberg chain have been presented. We have obtained the phase boundary between the RD and the dimer phases on $u + \frac{W^2}{2} = 1$. We expect there would be a phase boundary line connecting $(W, u) = (0, 0)$ and $(1.46, 0.27)$ in the $W-u$ plane.

For $|u| < \frac{W^2}{2}$, the bond distributions of odd and even bonds overlap with each other. Therefore, it is naturally expected that one could find a very long and almost clean segment with arbitrary small excitation gap. However, the present result clearly shows that the spin gap can survive even in such regions. Its proper interpretation remains as an open question.

For the $S = 1$ chain, similar behavior of the uniform susceptibility as in the case of $S = \frac{1}{2}$ dimerized chain has been found. Detailed analysis (critical strength of randomness, etc.) for this system is now being proceeded and will be presented elsewhere.

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