Randomness Effects on Quantum Phase Transitions of Bond-Alternating Haldane Chain

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1 Introduction

Recently, effects of disorder on low-dimensional quantum magnets have been investigated extensively in theoretical studies. Especially, non-magnetic impurity effects on spin-gapped Heisenberg antiferromagnets [1] have aroused much interest in relation to the impurity-induced antiferromagnetic long-range order observed experimentally in real materials [2]. It has been established by the recent numerical simulations [3,4] that in two dimensions or higher, there are two classes of disorder, which affect spin-gapped states in essentially different ways. The site dilution and the bond dilution are representatives of each class. The former induces localized moments around the impurity sites. There exist strong correlations between such effective spins retaining the staggeredness with respect to the original lattice, and therefore the antiferromagnetic long-range order emerges by an infinitesimal concentration of dilution. In the bond-dilution case, on the other hand, localized moments are always induced in pairs and they reform a singlet by the antiferromagnetic interactions through the two- or three-dimensional shortest paths as long as the concentration of bond dilution is smaller than a finite critical value.

In one-dimensional systems, since quantum fluctuations are much stronger than in the higher-dimensional cases, novel quantum critical phenomena are observed under disorder in the magnitude of coupling constants (bond randomness). Theoretically, the decimation renormalization group (RG) approaches have achieved great success to predict rich physics, such as the random-singlet (RS) phase, especially for the $S = \frac{1}{2}$ chains [5,6]. Recently, this technique has been extended to the higher-spin cases [7–10], where the main debate is on the robustness of the $S = 1$ Haldane phase [11] in the presence of disorder. A number of numerical studies have also been done [12–15] in order to establish the quantitative phase diagrams. However, this problem has not been made clear enough yet. One of the main difficulties in numerical simulations of random quantum systems is the extremely wide energy scale to be taken into account. Another difficulty is the lack of appropriate physical quantity to discuss the randomness-driven criticality effectively.

In this report, we present the results of our recent large-scale quantum Monte Carlo (QMC) studies on the ground-state properties of the bond-alternating Haldane chain with bond randomness [16]. In order to overcome the difficulties mentioned above, we introduce two novel numerical techniques, i.e. the ground-state loop algorithm [17] and the twist order parameter [18], in the present QMC simulation. After introducing our model in Sec. 2, in the succeeding sections we give brief overviews on the techniques we use in our simulation. In Sec. 5, our QMC results are presented and the phase diagrams are compared to those by the previous studies. We give a summary and discussions on the present results in the final section.

2 Model

We consider the antiferromagnetic Heisenberg chain described by the following Hamiltonian:

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

where $\mathbf{S}_i$ is a spin operator at site $i$ with $\mathbf{S}_i^2 = S(S + 1)$. The system size is given by $L$. 
and periodic boundary conditions are assumed ($S_{i+L} = S_i$).

For the pure bond-alternating model, the coupling constants $\{J_i\}$ are given by

$$J_i = 1 - \delta(-1)^i .$$

The parameter $\delta (|\delta| \leq 1)$ controls the strength of bond alternation (or forced dimerization). The ground-state phase diagram of the pure model has been established in terms of the valence-bond solid (VBS) picture [19]. The configuration of the valence bonds $(m,n)$, where $m$ (n) denotes number of valence bonds on the odd (even) bonds, changes from $(0,2S)$ to $(2S,0)$ successively as $\delta$ is increased from $-1$ to 1, meaning the existence of 2S quantum phase transitions [20]. For the $S = \frac{1}{2}$ system, $\delta = 0$ is the critical point between the $(0,1)$ and $(1,0)$ VBS phases, while $\delta_c = \pm 0.25997(3)$ is obtained for the $S = 1$ system by the recent QMC calculation [18].

In the following, we consider two different random distributions for the couplings $\{J_i\}$. The first one is the uniform distribution, where the coupling constants are given by

$$J_i = [1 - \delta(-1)^i] \, r_i$$

with quenched random numbers $\{r_i\}$, distributed uniformly by

$$P(r_i) = \begin{cases} 1/2W & \text{if } |r_i| \leq W \\ 0 & \text{otherwise.} \end{cases}$$

Here $0 \leq W \leq 1 - |\delta|$ must be satisfied, so that all the couplings remain antiferromagnetic. The second one is the power-law distribution:

$$J_i = [1 - \delta(-1)^i] \, t_i$$

with $t_i$ obeying

$$P(t_i) = \begin{cases} R^{-1}t_i^{1+1/R} & \text{if } 0 < t_i \leq 1 \\ 0 & \text{otherwise,} \end{cases}$$

where the parameter $R$ is non-negative, and the $R = 0$ limit corresponds to the pure case ($t_i = 1$ for all $i$). Note that at $\delta = 0$ the uniform distribution (Eqs. (3) and (4)) with $W = 1$ and the power-law distribution (Eqs. (5) and (6)) with $R = 1$ are essentially the same besides a trivial scaling factor. That is, $J_i$ distributes uniformly between 0 and a finite cutoff in both cases.

### 3 Ground-State QMC Algorithm

The recently developed continuous-imaginary-time loop algorithm is one of the most efficient methods for simulating quantum spin systems [21, 22]. It is based on the world-line Monte Carlo method using the path-integral representation by means of the Suzuki-Trotter mapping [23]. In contrast to the conventional local-update QMC method, the continuous-imaginary-time loop algorithm works directly in the imaginary-time continuum, and thus is complete free from the systematic error due to the Suzuki-Trotter discretization. In addition, the correlation between successive spin configurations is greatly reduced even at low temperatures and/or near the critical points, sometimes by orders of magnitude. This is due to the fact that clusters of spins (or loops), each of which is flipped at once, have a typical linear size corresponding directly to the relevant spin fluctuations.

The loop algorithm works at finite temperatures. Since in the present study we are interested in the ground-state properties of the random spin chains, it is required a proper extrapolation scheme for taking the zero-temperature limit. Conventionally one performs QMC calculations at different temperatures and check if the physical quantities of interest at two neighboring low temperatures coincide or not. If not, another QMC simulation at a lower temperature is performed. This procedure will be repeated until the physical quantities converges to a finite value. This ‘temperature-lowering’ extrapolation has the following shortcomings: First, since the QMC data fluctuate statistically, they could accidentally coincide even in the high-temperature regime. Second, some physical quantities, such as the static structure factor at $k = \pi$ of the spin-gapped systems, may exhibit non-monotonic temperature dependence. Thus one needs QMC simulations at several temperatures to judge the convergence correctly.

Furthermore, there are other difficulties specific to the random systems. For such systems we need to average the physical quantities over several hundreds or thousands of samples (or realizations), and in general the values them-
selves as well as their convergence (saturation) temperature fluctuate strongly from sample to sample. Conventionally, one takes random average at certain fixed temperatures, then extrapolates to the zero temperature limit by the procedure described above. In this procedure, one will encounter large statistical fluctuations at each temperature, since the sample-to-sample fluctuations are much larger than the statistical error in each sample, and thus it will be very hard to check the convergence. The other way is taking random average after extrapolating each samples to their ground state. In this case, it will take vast amount of time and effort in checking the convergence of thousands of samples separately.

In order to overcome these difficulties, we proposed the ground-state loop algorithm [17]. First of all, it should be noticed that the ground state of the antiferromagnetic Heisenberg chain of even number of spins is always singlet, and there is a finite gap above the unique ground state as long as the system size is finite. The inverse of the gap is given by the correlation length in the imaginary-time direction in the path-integral representation. Since the loop size is directly related to the correlation length in the real-space as well as the imaginary-time directions, the system can not distinguish whether the temperature is finite or zero, if no loops wrap around the lattice in the imaginary-time direction. In other words, the winding number of the loops in the imaginary-time direction can be used as a good measure for the convergence to the ground state.

The idea explained above is easily implemented as a ground-state QMC algorithm as follows: We start at a certain temperature. At each Monte Carlo step, the winding number of the loops is measured. If at least one loop wraps around the system in the imaginary-time direction, we double the inverse temperature. This procedure will automatically adjust the simulation temperature so that the system will be at the ground state effectively.

Another implementation of the ground-state QMC algorithm is also possible [17]. In the second implementation, the system size in the imaginary-time direction is assumed infinite from the first. We always start constructing loops from the zero imaginary time ($\tau = 0$). Once all the loops originating from the zero imaginary time close, then flip these loops and proceed to the next Monte Carlo step. This version of the ground-state loop algorithm is an extension of the infinite-size single-cluster algorithm recently proposed by Evertz and von der Linden [24]. This algorithm can be implemented more efficiently in the stochastic series expansion (SSE) representation [25] instead of the path-integral one.

In the present calculation, we used the first variant of the ground-state algorithm. The detailed comparison of these two variants will be published elsewhere [17].

Before closing this section, we would like to emphasize the advantages of our present method over the other ground-state QMC algorithms, such as the Green-function Monte Carlo method [26]. It is well known that they suffer from serious critical slowing down and also from the so-called population control problem. On the other hand, the present algorithm has no such problems and thus it is much more efficient, since it is based on the cluster update.

4 Twist Order Parameter $z_L$

The successive phase transitions in the pure bond-alternating Heisenberg chain can be understood as a reconfiguration of valence bonds as explained in Sec. 2. Each VBS state has a topological hidden order and is characterized by means of the string order parameter. For example, for the $S = 1$ chain the following string order parameter has a finite value in the Haldane phase ($|\delta| < 0.25997(3)$), which belongs to the same class as the (1,1) VBS phase [27]:

$$O_{str} = - \lim_{|k-\ell| \to \infty} \langle S^z_k \exp[\pi \sum_{j=k+1}^{\ell-1} S^z_j S^z_\ell] \rangle. \quad (7)$$

The string order parameter can be generalized to the cases with $S > 1$ [20].

On the other hand, Affleck and Lieb studied the Haldane’s conjecture by the Lieb-Schultz-Mattis (LSM) type argument [28]. However, relation between the LSM argument and the
VBS picture including the string order parameter has not been fully understood. Recently, Nakamura and Todo has shown that the ground-state expectation value of the unitary operator appearing in the LSM argument plays a role of an order parameter characterizing the VBS states directly [18]. The unitary operator rotates all the spins about the z axis with a relative rotation angle $2\pi/L$ and thus it generates a low-lying excited state with the excitation energy of $O(L^{-1})$. The twist order parameter $z_L$ measures the overlap between the ground state and the twisted excited state; $z_L = 0$ means the existence of gapless excitations or the degenerating ground states. Furthermore, it is shown that in the $(m, n)$ VBS state $z_L$ converges to $(-1)^m$ in the thermodynamic limit. Thus, the twist order parameter detects the valence-bond configuration directly.

In Fig. 1, the twist order parameter $z_L$ is plotted as a function of $\delta$ for the pure bond-alternating chains with $S = \frac{1}{2}$, 1, $\frac{3}{2}$, and 2. As clearly seen, $z_L$ changes the sign $2S$ times respectively, corresponding the quantum phase transitions between the VBS states. By extrapolating the point where $z_L = 0$, one can estimate the critical point $\delta_c$ accurately. For example, $\delta_c = 0.25997(3)$ is obtained for the $(1,1)-(2,0)$ transition of the $S = 1$ chain [18]. Compared to the conventional string order parameter (7), the twist order parameter $z_L$ has many advantages. First, the twist order parameter is universal and applicable to many systems without modification, while different string order parameter should be introduced depending on the system under consideration. Second, by means of the twist order parameter it is possible to estimate the critical point more accurately, since $z_L$ changes the sign at the transition.

In Fig. 1, the twist order parameter $z_L$ is plotted as a function of $\delta$ for the pure bond-alternating chains with $S = \frac{1}{2}$, 1, $\frac{3}{2}$, and 2. The system size is $L = 64$. The point where $z_L$ changes its sign gives an estimate for the critical point (from Ref. [18]).

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system is driven to the RS phase. In this phase, there is also no excitation gap, but the correlation function decays with a different exponent from that of the pure system [5]. The RS phase is characterized by the infinite dynamical exponent $z$, i.e., a logarithmic scaling of the length scale and the energy scale. As a result, the uniform susceptibility diverges as

$$\chi \sim \frac{1}{T \log^2(T/T_0)}$$  \hspace{1cm} (11)$$

at low temperatures, where $T_0$ is a non-universal constant. These theoretical predictions have been confirmed by the recent numerical studies [29].

The RS phase is unstable against small bond alternation, and the real-space correlation becomes short ranged immediately [6,29]. On the other hand, the spin gap remains vanished up to a finite strength of bond alternation. This phase is referred to as the quantum Griffiths (QG) phase. In the QG phase, the uniform susceptibility obeys a power low ($\chi \sim T^{-\gamma}$) at low temperatures with a non-universal exponent $\gamma$.

In Fig. 2, the twist order parameter is plotted as a function of $\delta$ for the random $S = \frac{1}{2}$ chain with the power-law random distribution ($R = 0.5$). The twist order parameter with different system sizes crosses at $\delta = 0$ clearly. Note that in the random system, the translational and the parity symmetries are both broken in each sample, and thus $z_L$ does not necessarily become zero at $\delta = 0$. However, one sees in Fig. 2 that these symmetries are restored after the random average is taken. For a non-zero $\delta$, the twist order parameter quickly converges to $\pm 1$ depending on the sign of $\delta$, though it is known that there extend the gapless QG phases at the both sides of the RS point ($\delta = 0$) [6, 29]. These results demonstrate that the twist order parameter $z_L$ does not affected by the QG singularity and it is effective to detect the RS critical point as a crossing point, as the same as for the pure systems.

5.2 Spin-1 chain with uniform distribution

Next, we consider the $S = 1$ system with the uniform bond distribution (Eqs. (3) and (4)). At $\delta = 0$ and without randomness, the system has a finite gap and a finite correlation length [11]. By the previous RG studies, it is predicted that this Haldane state is stable against weak disorder, while there occurs a quantum phase transition to the $S = 1$ RS phase at a critical strength of randomness. By the previous QMC analysis on the uniform susceptibility and the string order parameter [14], it is indicated that the phase transition occurs at $W \simeq 0.95$. However, in the present calculation, the twist order parameter decreases in the whole range of $W$ ($0 \leq W \leq 1$) with increasing the system size, and tends to converge to -1 without any crossing, indicating that the

Figure 2: $\delta$ dependence of the twist order parameter $z_L$ for the $S = \frac{1}{2}$ system with $R = 0.5$. At $\delta = 0$, $z_L$ is zero irrespective of the system size, while it converges to $\pm 1$ for $\delta \neq 0$.

Figure 3: Phase diagram of the $S = 1$ system with the uniform bond distribution. On the $\delta = 0$ line, the Haldane phase survives up to $W = 1$. 

Note that in the random system, the translational and the parity symmetries are both broken in each sample, and thus $z_L$ does not
Haldane ((1,1) VBS) phase is robust against the disorder in the whole range of $W$.

This can be seen more clearly in the $\delta$-$W$ phase diagram. The $S = 1$ chain has a ground-state phase diagram qualitatively different from that of the $S = \frac{1}{2}$ one. In the pure system ($W = 0$) the Haldane phase existing at $|\delta| < 0.25997(3)$, and this region is considered to shrink as the strength of randomness increases [9].

In Fig. 3, we show the $\delta$-$W$ phase diagram of the $S = 1$ system with uniform distribution obtained from the crossing point of the twist order parameter with different system sizes ($L = 8, 16, 32, 64$). For small $\delta$, the phase diagram we obtained is qualitatively the same as the one predicted by the RG study [9]. However, the phase boundary (solid line) between the Haldane (1,1) and the dimer (2,0) phases merges with the line denoting $\delta + W = 1$ (dashed line), and does not reach $\delta = 0$ even at $W = 1$. Indeed the critical point along $\delta + W = 1$ is estimated as $\delta \simeq 0.1$. Thus, we conclude that there is no $S = 1$ RS phase at $\delta = 0$ in the present model.

### 5.3 Spin-1 chain with power-law distribution

In this subsection, we examine the other distribution for the random couplings, i.e., the power-law distribution (Eqs. (5) and (6)). As already pointed out in Sec. 2, the power-law distribution with $R = 1$ is equivalent to the uniform distribution with $W = 1$, and thus it is expected that the Haldane phase is stable at least up to $R = 1$ also for the power-law distribution. However, one can consider further disorder ($R > 1$), i.e. a wider distribution in a logarithmic scale, in the present case, by which the Haldane phase might be broken.

In Fig. 4, the twist order parameter is plotted as a function of $\delta$ in the weak randomness regime ($R = 0.5$). As one can see clearly, for $\delta > 0.2$, the twist order parameter increases as the system size increases and tends to converge to +1. We identify this phase as the dimer (2,0) phase. On the other hand, $z_L$ tends to converge to -1 for $\delta < 0.2$, indicating the Haldane (1,1) phase. As expected, the phase diagram at $R = 0.5$ is quite similar to the one at $W = 0.5$ ~ 0.6 in the case of uniform distribution (Fig. 3).

At the crossing point $\delta \simeq 0.2$, a quantum phase transition occurs from the Haldane phase to the dimer phase, and the transition is expected to belong to the $S = \frac{1}{2}$ RS universality class [9]. In order to confirm this prediction, we measured the distribution of the local susceptibility

$$\chi_{loc, i} = \beta \langle m_i^2 \rangle = \int_0^\beta d\tau \langle S_i^z(0) S_i^z(\tau) \rangle$$

at the critical point $(R, \delta) = (0.5, 0.2)$. As seen in Fig. 5, the distribution function of the logarithm of local susceptibility is scaled fairly well by assuming the following logarithmic scaling

$$P(\log \chi_{loc}) \simeq \tilde{f}(\log \chi_{loc} / L^\psi)$$
with $\psi = 0.42$. This is consistent with the previous RG prediction for the RS phase [5], though the value of the exponent $\psi$ is slightly smaller than the theoretical prediction ($\psi = 1/2$). This is a further support of applying the twist order parameter to the randomness-driven quantum phase transitions.

Repeating similar analyses, we obtain the whole $\delta$-$R$ phase diagram of the $S = 1$ random chain with the power-law distribution (Fig. 6). Similar to Fig. 3, the Haldane phase tends to shrink as $R$ increases. We confirm that it remains at least up to $R = 1$ as concluded in the previous subsection.

In contrast to the case of box distribution, however, the overall shape of the phase boundaries indicates the existence of the multicritical point, where the two critical lines merge with each other. To locate the multicritical point precisely, we calculate $z_L$ for several system sizes ($L = 16, 24, 32, 48, 64$) along $\delta = 0$. The results for $0.9 \leq R \leq 1.2$ is shown in Fig. 7, where the data with different system sizes crosses at $R_c = 1.05$ clearly. Thus, we conclude there exists a multi-critical point at $(R, \delta) = (1.05, 0)$, which is indicated by a solid square in Fig. 6. Below the multi-critical point the Haldane phase survives, though the spin gap vanishes at a certain $R (< R_c)$, where a crossover from the gapped Haldane phase to the gapless Haldane (or QG) one occurs. In the case of box distribution, the crossover is observed at $W \simeq 0.7$ [29], while we have not yet examined the crossover in detail for the power-law distribution. For $R > R_c$, on the other hand, the twist order parameter is expected to converge to zero in the thermodynamic limit, where the $S = 1$ RS phase is realized according to the previous RG analyses [7–9].

6 Summary and Discussions

In the present article, we reported the results of our large-scale QMC simulations on the bond-alternating random Haldane chain [16]. By introducing the two techniques, the ground-state loop algorithm and the twist order parameter, we have obtained successfully the precise phase diagram of the random spin chain. Especially we demonstrated that the twist order parameter, introduced originally for the pure spin chains, is quite effective also for the random systems.

For the uniform distribution, the present result, i.e. the absence of the $S = 1$ RS phase, does not agree with the previous QMC result, in which a multi-critical point was suggested [14]. A possible reason of the disagreement is that for random systems, rare and low energy scale but very strong correlations are very important, and the finite-temperature QMC method used in the previous study could fail easily to take such contributions into account correctly. On the contrary, in the ground-state loop algorithm proposed in the present study, the simulation temperature is automatically adjusted depending on the gap of each sample, so that the physical quantity at the zero temperature is calculated.
at an optimal cost. This algorithm is quite useful not only for simulating random systems, but also for the ground-state problems of non-random systems.

For the power-law distribution, on the other hand, we obtained the phase diagram with a multi-critical point, where the two $S = \frac{1}{2}$ critical RS lines merge together into the $S = 1$ RS line. The location of the multi-critical point was also determined accurately by using the twist order parameter. The phase diagram we obtained is consistent with the recent RG prediction [9], and thus the present results strongly support the validity of the RG analysis for the $S = 1$ systems. By the RG analysis, it is further predicted that the $S = \frac{1}{2}$ and the $S = 1$ RS critical lines in the phase diagram both belong to the same universality class, while the multi-critical point exhibits different critical behavior. In addition, more rich phase diagrams have been obtained for higher-spin systems ($S \geq \frac{3}{2}$) [9]. It is an interesting future problem to confirm the universality/non-universality of the RS criticality as well as the RG phase diagrams for the higher-spin systems in terms of the present numerical techniques, the ground-state loop algorithm and the twist order parameter, which can be applied straightforwardly to such systems.

References

[23] For reviews, see e.g., Quantum Monte Carlo Methods in Condensed Matter Physics, ed. M. Suzuki (World Scientific, Singapore, 1994), and references therein.