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Stability of the Haldane state against the antiferromagnetic-bond randomness

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Abstract. Ground-state phase diagram of the one-dimensional bond-random $S = 1$ Heisenberg antiferromagnet is investigated by means of the loop-cluster-update quantum Monte-Carlo method. The random couplings are drawn from a rectangular uniform distribution. We found that even in the case of extremely broad bond distribution, the magnetic correlation decays exponentially, and the correlation length is hardly changed; namely, the Haldane phase continues to be realized. This result is accordant with that of the exact-diagonalization study, whereas it might contradict the conclusion of an analytic theory founded in a power-law bond distribution instead. The latter theory predicts that a second-order phase transition occurs at a certain critical randomness, and the correlation length diverges for sufficiently strong randomness.

PACS. 75.10.Jm Quantized spin models – 75.10.Nr Spin glass and other random models – 75.40.Mg Numerical simulation studies

1 Introduction

In *quantum* statistical mechanics, the effect of randomnesses remains non-trivial, even though they do not introduce any frustrating interactions. From the path-integral point of view, random quantum system is regarded as a certain classical system, where the randomness distributes along the real-space directions, while the interaction along the imaginary-time direction is fixed to be uniform. Hence, it is expected that the anisotropy between the real-space and the imaginary-time directions would cause an exotic phase which has not yet been found in the studies of classical random systems [1]. In fact, the ground-state magnetic transition of the random transverse Ising model shows a significant anisotropy between these directions [2–4]. The anisotropy results in an unique critical phenomena, where the dynamical critical exponent diverges at the transition point.

It would be notable that the above example is merely of one-body problem, because the one-dimensional transverse Ising model is transformed to the *free* spinless fermion model with the Jordan-Wigner transformation. Random *many-body* systems would be more exotic, and have been attracting considerable attention recently. In particular, the one-dimensional $S = 1/2$ random Heisenberg chain has been studied for such randomnesses as the random magnetic field [5–7], the random bond [8,9] and the X-Y-symmetric random exchange [6,10]. Various theoretical methods, that is, the real-space decimation method, the bosonization technique and the numerical simulation, have been employed in these studies. In the case of the random bond, the real-space decimation method [11,12] is particularly useful, and yields comprehensive understanding of the system [8]: it was found that the so-called random-singlet phase is realized for the infinitesimal amount of the bond randomness; see the phase diagram in Figure 1a. In the random-singlet phase [6,8], the spin-correlation decays in the form $\sim 1/r^2$ (note that without any randomnesses it decays as $\sim 1/r$), and the magnetic susceptibility diverges in the form,

$$\chi(T) \sim \frac{1}{T \log^2(\Omega/T)}, \tag{1}$$

at low temperatures (the parameter Ω denotes the width of the random-bond distribution). It is noteworthy that the susceptibility diverges at low temperatures, even though the ground state is off-critical. This singularity is known as the Griffiths-McCoy singularity [16,17], which was first proposed for the dynamics of classical random systems.

It is suggestive that the real-space decimation method fails for the cases other than $S = 1/2$. Its failure is reasonable in the sense that the ground state properties are different qualitatively between the half-odd-integer- and the integer-spin chains. This difference was conjectured theoretically by Haldane [18]. He claimed that the integer (half-odd-integer) spin chain shows massive (gapless) magnetic excitation above the ground state, and the magnetic correlation decays exponentially (obeying the power law) in the ground state. The massive magnetism, such as the ground state of the $S = 1$ Heisenberg chain, is beyond

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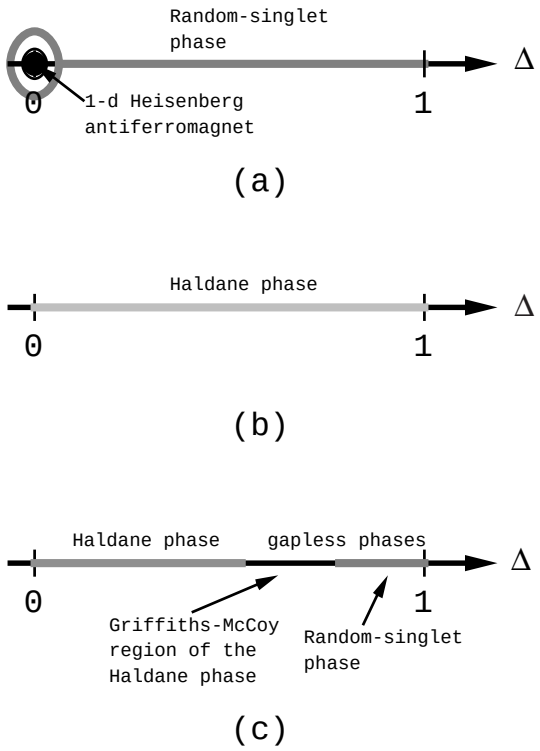

Fig. 1. Ground-state phase diagrams for the bond-random antiferromagnetic chain proposed so far. (a) The diagram for the $S = 1/2$ chain determined with the real-space renormalization group method [8] and the bosonization technique [6]. This conclusion is fairly established. (b) The same diagram but for the $S = 1$ magnet concluded in the present work and the previous exact-diagonalization study [13]. (c) The same as (b) but was determined with the real-space-decimation method [14,15]. The interpretation of the result in terms of ours is not straightforward, because the method uses a power-law bond distribution instead.

the scope of the previous analytic techniques, and is of current interest [13,14,19,20].

Here, we study the one-dimensional bond-random $S = 1$ antiferromagnet whose Hamiltonian is given by,

$$\mathcal{H} = \sum_{i=1}^{L} J_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}. \tag{2}$$

The operators $\{\mathbf{S}_i\}$ denote the $S = 1$ spin operators acting on the site i. The periodic boundary condition $\mathbf{S}_{L+1} = \mathbf{S}_1$ is imposed. The bonds $\{J_i\}$ are distributed independently with respect to the probability distribution, see Figure 2,

$$P_{\Delta}(J) = \frac{1}{2\Delta}(\Theta(J - 1 + \Delta) - \Theta(J - 1 - \Delta)). \tag{3}$$

(The function $\Theta(x)$ denotes the step function.) The parameter Δ governs the strength of the randomness. The randomness $\Delta = 1$ describes the case of the extremely broad bond distribution, where infinitesimally weak bond may appear. We have investigated the Hamiltonian with the quantum Monte-Carlo method with use of the loop-cluster-update algorithm [21]. The loop-cluster-update algorithm is efficient especially at low temperatures.

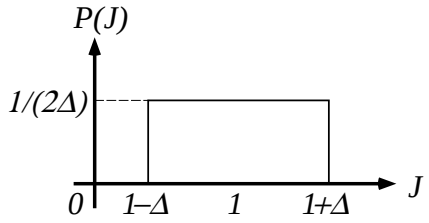

Fig. 2. The probability distribution of the bond strength $\{J_i\}$. The randomness ranges as $0 \leq \Delta \leq 1$. At $\Delta = 1$, the distribution becomes extremely broad; namely, infinitesimally weak bond appears.

We show that even for extremely broad bond distribution such as $\Delta = 0.9$, the magnetic correlation length continues to be unchanged. Namely, the long-range correlation is not affected by the randomness. The result indicates the stability of the Haldane state against the randomness; see our phase diagram in Figure 1b. This conclusion supports the suggestion of the previous exact-diagonalization study [13] by the present author, while it might be rather inconsistent with the analytical theories [14,15]. (It is not so straightforward to interpret the result in terms of ours, because in the theories, a power-law bond distribution is used, whose distribution is broader than ours.) These theories state that for sufficiently strong randomness, gapless phases such as the Griffiths-McCoy and the random-singlet phases would appear; see Figure 1c. The exact-diagonalization method has an advantage that we can simulate the ground-state eigenstate directly, although the tractable system size $L = 14$ is rather limited. We stress that the present Monte-Carlo analysis treating system sizes up to $L = 64$ compensates our previous exact-diagonalization study [13].

The present paper is organized as follows. In the next section, details of our simulation and the numerical results are presented. In the last section, we give summary and discussions.

2 Numerical results

In this section, we investigate the ground-state phase diagram of the Hamiltonian (2) numerically. We focus on the situation of very strong randomness $\Delta \sim 1$.

2.1 Details of the numerical simulation

We have employed the quantum Monte-Carlo method with the loop-cluster-update algorithm [21]. The loop-cluster algorithm was first proposed for the $S = 1/2$ magnet, see the article [22] for a review. The algorithm for the case $S = 1$ was formulated in the article by Kawashima [23]. We followed his formulation: as in the conventional quantum Monte-Carlo method, the quantum system (2) is mapped to a classical spin system with the Suzuki-Trotter decomposition [24]. The spin flip of the resultant classical system is proceeded in a global manner. At each Monte-Carlo step, all the spins are decomposed into clusters,

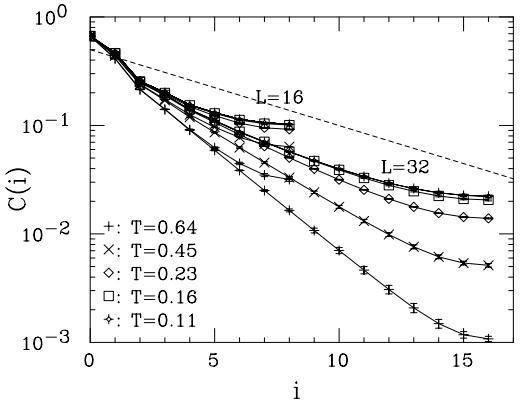

Fig. 3. Plot of the magnetic correlation for $\Delta = 0$ and the system sizes $L = 16$ and 32. The dashed line shows the decay of the correlation length $\xi = 6.2$ estimated previously [26].

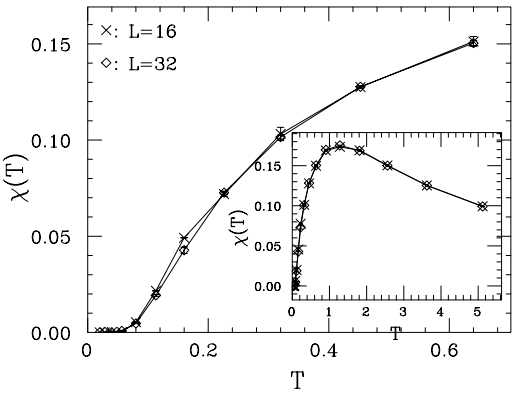

Fig. 4. Plot of the magnetic susceptibility for $\Delta = 0$. The inset shows the susceptibility for wider range of temperature.

and the spins belonging to an identical cluster is either flipped or un-flipped simultaneously with the probability $p = 0.5$.

The loop-cluster scheme reduces the autocorrelation time considerably. It is reported [25] that for the pure $S = 1$ Heisenberg chain, the autocorrelation becomes $10^2 \sim 10^4$-times shorter than that of the conventional local update method. Moreover, the autocorrelation time is independent on the Trotter number, and remains of the order unity. This advantage enables us to simulate at low temperatures without consuming huge Monte-Carlo steps. Owing to this, even at very low temperatures, we could concentrate on the average over the random samples rather than the estimation of the thermal averages for each sample.

Throughout the present study, we simulated 200 random samples, and for each sample we generated 10^4 Monte-Carlo steps – preceded by the 10^3 initial updates – so as to evaluate thermal averages. These sets of simulations are carried out for the Trotter numbers $N = 64$, 96 and 128. The final plots shown below are those extrapolated for $N \to \infty$ with use of these three data.

2.2 Numerical results for the pure magnet $\Delta = 0$

We present the results for $\Delta = 0$; that is, the case without any randomnesses. These results should be contrasted with those in the presence of the randomness $\Delta \neq 0$ shown afterwards.

In Figure 3, we show the logarithmic plot of the magnetic correlation $C(i)$ for various temperatures;

$$C(i) = \langle S_1^z S_{1+i}^z \rangle. \tag{4}$$

Here, the bracket $\langle \cdots \rangle$ denotes the thermal average. We observe that the correlation decays exponentially, and the correlation length develops as the temperature decreases. Even at very low temperatures, the magnetic correlation decays exponentially. That is, the magnetism is disordered even at the ground state: this behavior is consistent with the prediction by Haldane [18] as is introduced in the previous section. The correlation length and the magnetic excitation gap are estimated numerically as $\xi = 6.2$ and $\Delta E = 0.41049(2)$ [26], respectively. The correlation length in Figure 3 is accordant with this estimate. In Figure 4, we plotted the the susceptibility $\chi(T)$ against the temperature T. Our result recovers the plot appearing in the article [27]: at high temperatures, the susceptibility increases as the temperature decreases following the Curie law $\chi(T) \propto 1/T$ On the contrary, bellow the temperature $T \sim 1$, the susceptibility becomes suppressed rapidly. This suppression is common to the magnetism with magnetic excitation gap. The drop-down temperature indicate the magnitude of the excitation gap; note that the Haldane gap mentioned above and the suppression temperature in Figure 4 are comparable.

2.3 Results for strong randomness $\Delta \sim 1$

First, we show the results for the very broad bond distribution $\Delta = 0.9$. In Figures 5 and 6, we presented the log and log-log plots of the magnetic correlation $C_{av}(i)$, respectively;

$$C_{av}(i) = [\langle S_1^z S_{1+i}^z \rangle]_{av}, \tag{5}$$

where the bracket $[\cdots]_{av}$ denotes the random-sampling average. As is shown in the figures, the long-range form of the correlation apparently suits the exponential form rather than the power-law one: in the log plot in Figure 5, the correlation-function data form a straight line for a wide range of the distance i. In the log-log plot in Figure 6, on the contrary, the data are curved. In the latter figure, we showed the decay form $\sim 1/r^2$ as a dashed line whose form should be realized in the random-singlet phase. We see no such sector that is fitted by the dashed slope.

We conclude that the magnetic correlation decays exponentially even for very broad bond distribution. Moreover, the correlation length is kept hardly changed; compare Figure 5 with Figure 3. (We observe that the

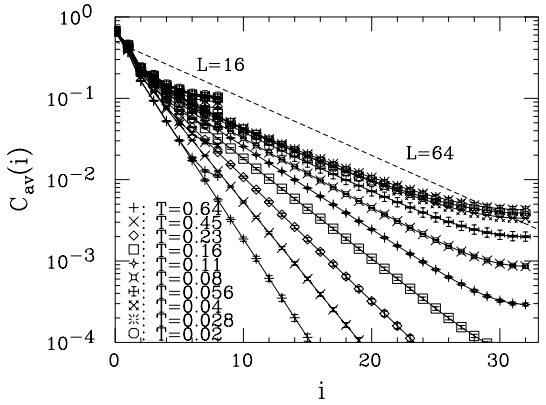

Fig. 5. Logarithmic plot of the magnetic correlation for $\Delta = 0.9$ and the system sizes $L = 16$ and 64. The dashed line indicates the decay rate $\xi = 6.2$ [26], which describes asymptotic form for the system $\Delta = 0$.

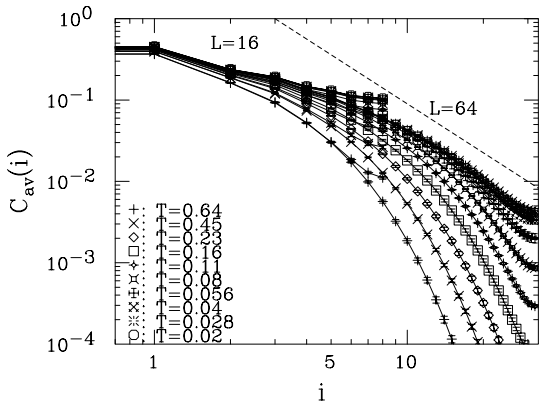

Fig. 6. Log-log plot of the magnetic correlation for $\Delta = 0.9$ and the system sizes $L = 16$ and 64. We also show the decay form $\sim 1/r^2$ as a dashed line which should succeed in fitting the data for the random-singlet phase.

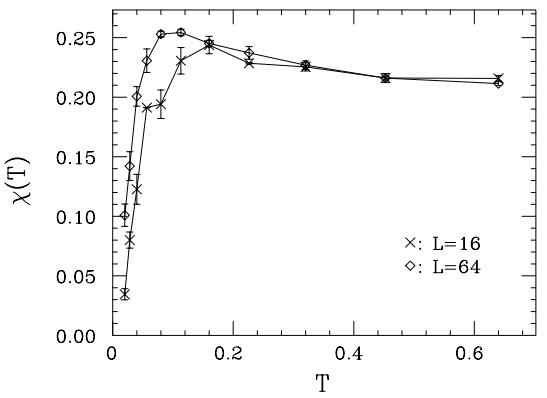

Fig. 7. Plot of the magnetic susceptibility for $\Delta = 0.9$.

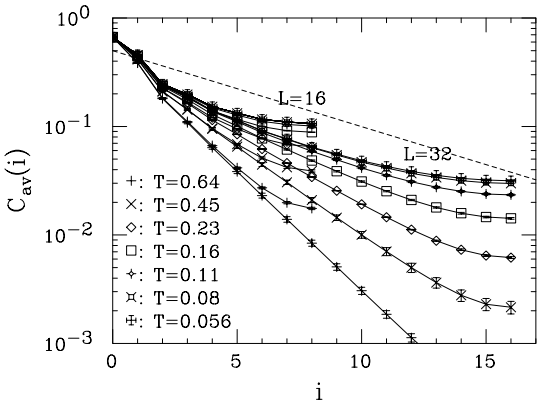

Fig. 8. Logarithmic plot of the magnetic correlation for $\Delta = 0.7$ and the system sizes $L = 16$ and 32. The dashed line indicates the decay rate $\xi = 6.2$ [26], which describes the asymptotic form for the system $\Delta = 0$.

correlation length is slightly stretched by the randomness. This stretch occurs only in the vicinity of the extreme point $\Delta = 1$. It would be interesting that the randomness contributes the magnetic order to be stabilized.) We found that the Haldane ground state is very stable against the randomness. Note that the analytic theory predicts that for sufficiently strong randomness, the correlation length should diverge [14,15]. The present result, however, indicates that the correlation length is not changed very much until at the extreme point $\Delta \to 1$.

As is shown above, the bond randomness does not influence the ground state properties very much. The susceptibility, on the other hand, suffers from the disorder; see Figure 7. We see that the susceptibility survives down to very low temperatures; compare this plot with that in Figure 4. The susceptibility starts to drop at $T \sim 0.1$. This result shows that the magnitude of the excitation gap is reduced considerably by the bond randomness. This tendency is understood as follows: as the randomness is turned on, the weak bonds of the strength $J_{min} \sim 1 - \Delta$ can appear; remind the probability distribution of the bond strength (3). Around the weak bond, the magnetic excitation, that is, the triplet magnon, costs the least energy of the order J_{min}, which is apparently smaller than that of the pure system $\sim J$. Because the excitation states are magnetic, the magnetic susceptibility survives down to the temperature J_{min}.

In fact, in Figure 7, we observe that the susceptibility starts to drop at $T \sim 0.1$, which is comparable to the estimate of the above argument $J_{min} \sim 0.1$. The crucial point to be noted here is that the excitation states are sensitive to the bond randomness, whereas the ground state is not.

Finally, we show the results for $\Delta = 0.7$; see Figures 8 and 9.

In Figure 8, we plotted the correlation function. The behavior of the correlation function is quite similar to those for $\Delta = 0$ and 0.9. Namely, even at very low temperatures, the correlation decays exponentially, and the ground-state correlation length is kept to be $\xi \sim 6.2$ as well. Surprisingly, the correlation-function data are quite similar to those for $\Delta = 0$, so that these are hardly

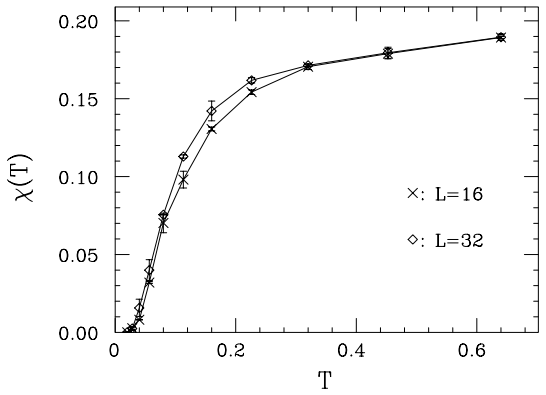

Fig. 9. Susceptibility is plotted for the randomness $\Delta = 0.7$ and $L = 16$ and 32

distinguishable. In fact, we found that these characteristics continue for the full range of the randomness. The above suggests the remarkable stability of the Haldane state against the bond randomness. We therefore propose the ground state phase diagram as in Figure 1b. In Figure 9, we plotted the susceptibility. The susceptibility drops rapidly below the temperature $T \sim 0.2$. This drop down temperature is higher than that for $\Delta = 0.9$; the magnetic excitation gap recovers to open as the strength of the randomness is reduced. We actually confirmed this tendency for various randomnesses, and that the variance is systematic. This fact seems to contradict to the picture shown in Figure 1c, where a singularity should occur at the transition point.

3 Summary and discussions

We have investigated the one-dimensional bond-random $S = 1$ antiferromagnet whose ground-state phase diagram has been controversial so far. We employed the quantum Monte-Carlo method by use of the loop-cluster-update algorithm [21,23]. The autocorrelation time of this update algorithm is much shorter than that of the conventual local update [23]. This advantage enables one to concentrate on the random sampling rather than consuming huge Monte-Carlo steps for the thermal averaging.

We have found that even at the very broad bond distribution $\Delta = 0.9$, the ground state is still in the Haldane phase with the correlation length kept hardly changed. Our data reveled the astonishing stability of the Haldane ground state against the bond randomness. On the contrary, the excitation levels are affected by the randomness severely. The magnetic excitation gap, namely, the Haldane gap, is found to be of the order of the weakest bond strength $\sim J_{min} = 1 - \Delta$. It closes as the randomness approaches to unity $\Delta \to 1$. To conclude, we propose the phase diagram as is depicted in Figure 1b.

The present result supports the conclusion of the previous exact-diagonalization study [13], whereas it might contradict to the analytic theory [14,15] which predicts that for sufficiently strong randomness, the ground state is in the random-singlet phase with diverging magnetic correlation length, see Figure 1c. (The analytic theory is founded in the power-law bond distribution, which is broader than ours. Hence, the correspondence might be not so straightforward.)

The exact-diagonalization study has a disadvantage that the tractable system size is rather limited ($L = 14$). Because our Monte-Carlo simulation, treating the system sizes up to $L = 64$, clarified that the correlation length remains unchanged $\xi \sim 6$, the system sizes treated in the exact-diagonalization study [13] are found to reach the scaling regime. The exact diagonalization enables us to access the ground-state eigenvector so as to yield various physical quantities such as the spin-stiffness constant. The spin stiffness is quite vital in studying the random systems. The stiffness was utilized successfully in the exact-diagonalization study [13]. We claim that the conclusion shown in Figure 1b is soundly established through combining the present Monte-Carlo simulation with the previous exact-diagonalization analysis [13].

The Haldane phase is realized in the AKLT model [28],

$$\mathcal{H}_{AKLT} = \sum_i J_i \left\{ \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3} (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \right\}, \qquad (6)$$

as well; the ground state, the so-called valence-bond-solid state, of the above Hamiltonian (6) is solved exactly. It is notable that the valence-bond-solid state is proved to be completely stable against the bond-randomness. Although the model is rather different from our Heisenberg Hamiltonian (2), we conjecture that the essence of the stability would be identical. This question should be solved in future.

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