Low Energy Properties of the Random Spin-1/2
Ferromagnetic-Antiferromagnetic Heisenberg Chain

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Abstract

The low energy properties of the spin-1/2 random Heisenberg chain with
ferromagnetic and antiferromagnetic interactions are studied by means of the
density matrix renormalization group (DMRG) and real space renormaliza-
tion group (RSRG) method for finite chains. The results of the two methods
are consistent with each other. The deviation of the gap distribution from
that of the random singlet phase and the formation of the large-spin state is
observed even for relatively small systems. For a small fraction of the ferro-
magnetic bond, the effect of the crossover to the random singlet phase on the
low temperature susceptibility and specific heat is discussed. The crossover
concentration of the ferromagnetic bond is estimated from the numerical data.
Keywords: random quantum Heisenberg chain, density matrix renormaliza-
tion group, real space renormalization group

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I. INTRODUCTION

Recently, the physics of random quantum spin chains has been attracting the broad interest of theoretical and experimental studies. It has been clarified that various exotic phases which are realized in neither regular quantum systems nor classical random systems appear in these systems. The interplay of quantum fluctuation and randomness is essential in understanding the low temperature thermodynamics of these systems.

The most widely used theoretical technique for this type of problem is the real space renormalization group (RSRG) method. In this approach, the distribution of the parameters such as the bond strength or the spin magnitude are renormalized step by step by changing the energy scale. The ground state phases are characterized by the fixed point distribution functions. In contrast to the RSRG method in the regular system, the RSRG method for the distribution function is often asymptotically accurate because of the broadness of the fixed point distribution. In the case of the random antiferromagnetic Heisenberg chain (RAFHC), it is known that the ground state is the random singlet (RS) phase in which the spins form singlets randomly not only with nearest neighbors but also with distant partners. Unlike the RVB state, however, the spatial pattern of the dimer covering is randomly fixed and does not fluctuate quantum mechanically.

The RSRG study of the random Heisenberg model with both ferromagnetic (F) and antiferromagnetic (AF) bonds (hereafter abbreviated as RFAFHC; random ferromagnetic-antiferromagnetic Heisenberg chain) has been carried out by Westerberg et al. Surprisingly, they predicted that this model belongs to a different universality class from the RS phase. In the presence of the ferromagnetic bonds, spins do not always die out but form large effective spins of various magnitude. Thus the fixed point is characterized by a fixed point distribution of the bond strength and spin magnitude even if the original system consists of only spins with magnitude 1/2. This type of ground state is called the large-spin phase.

On the other hand, the present author has introduced an algorithm which enables the application of the density matrix renormalization group (DMRG) method to the
random chains. [11] This method is applied to the RAFHC and gives results consistent with the RSRG theory. [8,11]

In the present work, the ground state and low energy properties of RFAFHC are investigated with the help of the DMRG and RSRG methods. In the next section, the Hamiltonian studied in this paper is presented. The numerical results are presented in section 3. The qualitative feature of the low temperature behavior and the crossover to the RS state in the limit of low F-bond concentration are discussed in section 4. In the last section, our results are summarized.

II. MODEL HAMILTONIAN

The Hamiltonian of the spin-1/2 RFAFHC is defined by

\[ H = \sum_{i=1}^{N} 2J_i S_i S_{i+1}, \quad |S_i| = 1/2, \]  

(1)

where \( J_i \) takes random values of both positive and negative signs. For the numerical calculation, we assume the following bond distribution \( P_0(J_i) \),

\[ P_0(J_i) = \begin{cases} 
\frac{1-p}{W} & 0 < J_{\text{min}} < J_i < J_{\text{max}}, \\
\frac{p}{W} & -J_{\text{max}} < J_i < -J_{\text{min}} < 0, \\
0 & \text{otherwise},
\end{cases} \]  

(2)

where \( W = J_{\text{max}} - J_{\text{min}} \). The absolute values of \( J_i \)'s are distributed uniformly between \( J_{\text{min}} \) and \( J_{\text{max}} \). The sign of \( J_i \) is F and AF with probability \( p \) and \( 1 - p \), respectively. Hereafter we set the energy unit by \( J_{\text{max}} = 1 \).

Furusaki et al. [9,10] investigated the finite temperature properties of the random exchange Heisenberg model with the \( \pm J \) bond distribution,

\[ P_0(J_i) = p\delta(J_i + J) + (1-p)\delta(J_i - J). \]  

(3)

This model is called \( \pm J \) Heisenberg chain (or \( \pm J \) HC) hereafter. The present model reduces to \( \pm J \) HC in the limit \( J_{\text{max}} \to J_{\text{min}} + 0 \). However there is a significant difference between
the present model and $\pm J$ HC in the limit $p \to 0$. Namely, in this limit, $\pm J$ HC reduces to the uniform spin-1/2 Heisenberg chain while the present model reduces to the RAFHC as long as $J_{\text{max}} \neq J_{\text{min}}$. Therefore the present model is suitable for investigating the crossover of the low energy properties of the RFAFHC to those of RAFHC as the concentration of the F-bond tends to 0.

III. NUMERICAL RESULTS

The algorithm of the DMRG calculation is essentially the same as that introduced in ref. [11]. In the present model, however, even the ground state is not always a singlet. Working in the subspace with $S_{\text{tot}}^z = 0$, the obtained target states generally have the finite total spin $S_{\text{tot}}$. In each step of renormalization, 2 spins are added. To obtain the low lying states of the superblock with $N + 2$ spins with $S_{\text{tot}}^z = 0$, the important states of the left and right blocks of the $N$ spin chain with $S_{\text{tot}}^z = \pm 1$ are taken into account, because the two additional spins can change $S_{\text{tot}}^z$ by $\pm 1$. The states with $S_{\text{tot}}^z = \pm 1$ are generated by the application of the ascending and descending operators of total spin $S_{\text{tot}}^\pm$ to the target state with $S_{\text{tot}}^z = 0$. This means that we have to keep three times the number of states compared to the case of the purely AF chain. In our calculation, we kept 140 states in each iteration step.

To compare the DMRG results with the RSRG results, we have also performed the RSRG calculation [7,8] for the finite systems. In contrast to Westerberg et al., [7,8] we do not add extra spins after each decimation. Therefore the effective length of the chain decreases step by step. The energy gap of the last step effective Hamiltonian is identified as the energy gap of the whole system. This procedure is performed for many samples and the gap distribution is calculated.

In the RS phase of RAFHC, the distribution of the logarithm of the energy gap $\Delta$ of the chain of length $N$ is scaled as $(\ln \Delta)/N^{1/2}$. [6] This implies that the average of ln $\Delta$ scales with $N^{1/2}$. This property is also confirmed to hold even for relatively small systems by the
DMRG method. On the other hand, according to Westerberg et al., the energy gap is scaled by the power of $N$ in RFAFHC as $\Delta \sim N^{-1/\delta}$ with $\delta \simeq 0.44$. In this case, the average of $\ln \Delta$ should scale with $\ln N$. This difference in the energy spectrum is reflected in the specific heat and magnetic susceptibility at low temperatures.

For the DMRG calculation, the number of samples ranges from 120 to 180 and the maximum system size is around 60. For the RSRG calculation, the number of samples is 2500. We have studied the cases of $p = 0, 1/5, 1/3$ and $2/3$ with $J_{\text{min}} = 0.5$ and $J_{\text{max}} = 1$. Figure 1 shows the system size dependence of the average $<\ln \Delta>$ plotted against $N^{1/2}$, which should be a straight line with a finite gradient for RAFHC, as in the case of $p = 0$. For $p = 2/3$, the deviation is significant even for the systems with $N \leq 60$ studied here. It should be noted that the results of RSRG and DMRG are consistent with each other as far as the $N$-dependence is concerned, although there is discrepancy in the absolute values for large $p$. The fact that the RSRG result concides semi-quantitatively with the DMRG result indicates the reliability of the RSRG results for larger systems, because the RSRG method becomes more and more accurate as the gap distribution broadens. Unfortunately, it is not possible to obtain the value of the exponent $\delta \simeq 0.44$ obtained by Westerberg et al. within the DMRG data. This means that the approach to the fixed point distribution is much slower than in the case of RAFHC for which the fixed point distribution is already reached for $N \leq 60$ within the DMRG data. Actually, Westerberg et al. used the chains of $10^5$ to $10^6$ sites to reach the fixed point distribution.

Figure 2 shows the system size dependence of the average of the square of the total spin magnitude $<S_{\text{tot}}^2>$. It is clearly seen that $<S_{\text{tot}}^2>$ is proportional to $N$ which is the specific feature of the large-spin phase of Westerberg et al. Here again the DMRG and RSRG data are consistent with each other. The ratio $c = <S_{\text{tot}}^2>/N$ is plotted against $p$ in Fig. 3. The solid line shows the fixed point relation $c = p/4(1-p)$ for $S = 1/2$. Thus our data show that the ground state is already clearly distinct from the RS ground state even for relatively small systems, although the approach to the true fixed point is extremely slow.
IV. CROSSOVER OF THE LOW ENERGY BEHAVIOR

The extremely slow convergence of renormalization flow prevents us from direct numerical investigation of the ground state of the present model especially for small $p$. Nevertheless, the crossover to the RS state in the limit $p \to 0$ can be speculated by combining our observations for the small systems and the analytical results obtained so far.

For small $p$, most of the spin pairs are connected by the random AF-bonds. In terms of the RSRG scheme, these spins are killed in the early stage of decimation leading to finite segments of the random singlet phase (RS segments) connected by the F-bonds. The energy gap distribution in the RS segment is given by the RS fixed point distribution function with finite energy cut-off $\Omega$ as 

$$P_{RS}(\Delta; \Omega) = \frac{\alpha}{\Omega} \left( \frac{\Omega}{\Delta} \right)^{1-\alpha} \theta(\Omega - \Delta),$$

with $\alpha = 1/\ln \Omega^{-1}$. The cut-off $\Omega$ and the exponent $\alpha$ is related to the size of the segment $N_S$ as

$$\ln(1/\Omega(N_S)) = \alpha(N_S)^{-1} \simeq C_0 + C_1 N_S^{1/2},$$

where $C_0$ and $C_1$ are numerical constants of the order of unity. The typical length of the RS segment is $1/p$ and its energy scale is $\Omega(1/p)$. The spins in the even-length RS segment can form complete random singlet states within each segment, while in each odd-length segment a spin-1/2 degree of freedom remains. These spin-1/2 degrees of freedom are coupled weakly via even-length RS segments with the effective bond strength of the order of $\Omega(1/p)$.

Based on the observation above, we can speculate the finite temperature behavior for small $p$, as schematically summarized in Fig. 4. In the intermediate temperature regime between the typical exchange energy of the original Hamiltonian and the cut-off energy of the typical RS segment $\Omega(1/p)$, the temperature $T$ determines the effective energy scale and the cut-off $\Omega(1/p)$ is irrelevant. Therefore the contribution to the susceptibility from the RS segments takes the usual RS form and gives the dominant contribution as
\[ \chi \sim \frac{\mu_B^2}{T |\ln^2 T|}. \] (6)

It should be noted that the spin-1/2 degrees of freedom in the odd-length AF segments gives the Curie-type contribution to the susceptibility \( \sim p/T \) because their number is proportional to \( p \). Nevertheless, the RS contribution is always dominant in this regime, because \( \ln^{-2} T \gg p \) as far as \( T \gg \Omega(1/p) \). The specific heat is similarly given by the RS form:

\[ C \sim \frac{1}{|\ln^3 T|}. \] (7)

This regime is denoted by I in Fig. 4.

As the temperature becomes lower than \( \Omega(1/p) \), distribution (4) with cut-off \( \Omega(1/p) \) gives the effective gap distribution in RS segments. At the same time, the spin-1/2 degrees of freedom in the odd-length segments start to be correlated. If the distribution \( P_{\text{RS}}(\Delta; \Omega(1/p)) \) is less singular than the universal fixed point distribution \( P_{\text{U}}(\Delta) \sim \Delta^{-y_c} \) with \( y_c \sim 0.7 \) obtained by Westerberg et al., then the renormalization flow will be attracted to this universal fixed point. This regime is denoted by regime II in Fig. 4. The susceptibility and the specific heat are given by,

\[ \chi \sim \frac{\mu_B^2 p}{12T(1 - p)}, \] (8)

\[ C \sim T^\delta \ln T \quad \text{with} \quad \delta \simeq 0.44, \] (9)

following refs. [7,8].

On the other hand, if the distribution \( P_{\text{RS}}(\Delta; \Omega(1/p)) \) is more singular than the universal fixed point distribution, the low energy physics is governed by the finite size RS distribution \( P_{\text{RS}}(\Delta; \Omega(1/p)) \) for the finite segments. Therefore, the specific heat is dominated by the finite size RS contribution,

\[ C \sim T^{\alpha(1/p)}. \] (10)

similarly to the case of random dimer phase [12]. However, the odd-length RS segments still involve the spin-1/2 degrees of freedom which contribute to the susceptibility.
that the effective magnitude of the cluster spin scales with the square of the cluster size even for the chains with singular initial bond distribution close to the RS fixed point distribution (chain E of ref. [8]), these spin-1/2 degrees of freedom would also contribute to Curie law susceptibility (8) in the similar way as in the universal case. This regime is denoted by III in Fig. 4. Physically speaking, the spin degrees of freedom in the RS segments die out as the temperature is lowered and therefore the contribution to the susceptibility is less singular than the Curie law. However, energetically, there remain arbitrarily weak singlet pairs in the RS segments which dominate the low temperature specific heat in this regime.

As \( p \to 0 \), the lower limit of the intermediate regime \( \Omega(1/p) \) tends to 0 and the RS behavior \( \chi \sim \mu_B^2/(T \ln^2 T) \) is recovered down to \( T = 0 \) in this limit. This is in contrast to the case of \( \pm J \) HC studied by Furasaki et al., [9,10] for which the thermodynamics at the intermediate temperature is described by the assembly of F and AF segments and approaches the uniform AF chain as \( p \to 0 \).

The critical concentration \( p_c \) between regimes II and III is determined by \( y_c = 1 - \alpha(1/p_c) \). The numerical value of \( p_c \) can be estimated from the DMRG data for \( p = 0 \) (RAFHC) as follows. The \( N \)-dependence of \( \alpha(N) \) can be deduced from the formula \( |< \ln \Delta >_{p=0}| /2 = \alpha(N)^{-1} \) verified by integrating (4). Fitting the DMRG data for \( p = 0 \) to (5), we find \( C_1 \simeq 0.3 \) (Fig. 4) while \( C_0 \) depends on the choice of the energy unit by definition. Although the energy unit was fixed by \( J_{\text{max}} = 1 \) in the beginning, here it is more appropriate to redefine the energy unit so that the relation \(- < \ln \Delta > /2 = \sigma \equiv < (\ln \Delta - < \ln \Delta >)^2 >^{1/2} \), which is valid for the distribution (1), holds for large enough \( N \). This leads to \( C_0 \simeq -0.78 \) and \( p_c \simeq 0.0053 \). This procedure is better than the direct fit to \( \sigma \) because the convergence of \( \sigma \) to the fixed point value is slower than \( < \ln \Delta > \). It would be quite difficult to access the region \( p < p_c \) by the DMRG method, because systems much larger than 190 (\( \sim 1/0.0053 \)) would be required for this purpose.
V. SUMMARY

The low energy properties of the random ferromagnetic-antiferromagnetic quantum Heisenberg chain with spin-1/2 is studied by means of the DMRG and RSRG methods. It is demonstrated that the RSRG scheme gives results consistent with those of DMRG even for relatively small systems, which confirms the accuracy of the RSRG scheme for larger systems. It is shown that the distribution of the logarithm of the gap deviates from that of the random singlet phase and \( < S^2_{\text{tot}} > \) grows with the system size indicating the transition to the large-spin phase. However, the size of the system tractable by the DMRG is too small to approach the fixed point. Based on the numerical and analytical results obtained so far, the physical picture of the crossover of the low energy behavior to the random singlet phase is discussed. The critical concentration of the F-bonds is estimated from the numerical data.

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FIGURES

FIG. 1. The system size dependence of the average $< \ln \Delta >$ plotted against $N^{1/2}$ for $p = 0, 1/5, 1/3$ and 2/3 with $J_{\text{min}} = 0.5$ and $J_{\text{max}} = 1.0$. The DMRG data for $p = 0$ are shown by $\times$. For $p \neq 0$, filled symbols are DMRG data and open symbols are RSRG data.

FIG. 2. The system size dependence of $< S_{\text{tot}}^2 >$ for $p = 1/5, 1/3$ and 2/3 with $J_{\text{min}} = 0.5$ and $J_{\text{max}} = 1.0$. Filled symbols and solid lines are DMRG data and open symbols and broken lines are RSRG data. The lines are the least squares fits to the data.

FIG. 3. The $p$-dependence of $c = < S_{\text{tot}}^2 / N >$ estimated from DMRG data ($\bullet$), RMRG data ($\circ$) and fixed point value $p/4(1 - p)$ by Westerberg and coworkers.[7,8](solid line).

FIG. 4. Schematical low temperature behavior of RFAFHC for small $p$. All lines are crossover lines. At $T = 0$, the ground state corresponds to the universal fixed point for $p > p_c$ and to the non-universal one for $p < p_c$. 