Real-Space Renormalization Group Study of Effects of Anisotropy on S=1 Random Antiferromagnetic Chain

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We investigate S=1 antiferromagnetic quantum spin chain, whose exchange couplings are strongly disordered. By the real-space renormalization group method, introduced by Ma, Dasgupta, and Hu, the renormalization group flows are analyzed numerically in a plain of the anisotropy of the exchange coupling vs. the staggered magnetic field. As the result, the Heisenberg point, which has a zero average of the exchange coupling anisotropy, is specified as the unstable fixed point against the anisotropy.

KEYWORDS: antiferromagnetic quantum spin chain, randomness, anisotropy, real-space renormalization group

§1. Introduction

As is well known, in one-dimensional S=1 antiferromagnetic Heisenberg (AFH) models, the ground state is quantumly disordered by the strong quantum fluctuation.1) There is a finite excitation gap above their non-degenerating ground state. Affleck et al. have exactly proved this fact for the model with biquadratic interactions, employing the valence-bond-solid (VBS) picture.2) The existence of the gap in the low-energy excitation makes the system robust against weak bond-randomness in the case with $J_{\text{min}} \gg \Delta$, where $J_{\text{min}}$ is the minimum bond strength in all and $\Delta$ is the magnitude of the excitation gap in the case without randomness.

However, when the randomness becomes stronger, i.e. $J_{\text{min}} \sim \Delta$, the situation can be changed. Two far separated spins can form a singlet state even if they destroy the excitation gap of the bulk system. If the system contains an as large VBS cluster as the system size, the string order parameter still has a finite value. But if not, the string order parameter may vanish. This transition from quantum Griffiths (QG) phase to random singlet (RS) phase has been investigated numerically by the exact diagonalization method,3) the density matrix renormalization group (DMRG)
calculation,\textsuperscript{4} the quantum Monte Carlo (QMC) simulation,\textsuperscript{5} and the real-space renormalization group (RSRG) method.\textsuperscript{10}

The RSRG method is convenient one to determine the explicit phase diagram in the ground state of a system with randomness. This method has been introduced by Ma, Dasgupta, and Hu to study the $S=\frac{1}{2}$ AFH chain,\textsuperscript{6} and developed to being applied to other systems both in the analytical way and the numerical one.\textsuperscript{7–16} Among these works, we should point out a very important one by Fisher.\textsuperscript{8} He has fully studied the properties of the $S=\frac{1}{2}$ antiferromagnetic chains with various types of random exchange coupling in the analytical RSRG method. Especially, he has concluded that the Heisenberg point is nothing but the unstable fixed point (XXX RS fixed point), at which there occurs a transition from the XX RS phase to the Z (Ising) antiferromagnetic (ZAF) phase in a random XXZ chain.

As pointed out afterward, the RSRG method has the defect when it is applied to $S \geq 1$ spin system.\textsuperscript{14} Therefore, we should take care to use it in such a way that few inadequate renormalization processes are involved. Some authors have created skillful procedures, such as the use of the effective Hamiltonian,\textsuperscript{9,13,15,16} and by keeping more degrees of freedom.\textsuperscript{10} However, these skillful procedures cannot be applied in a fully consistent way to models with uniaxial anisotropy. The uniaxial anisotropy arises inevitably when the renormalization process is executed in the $S \geq 1$ quantum spin system with the magnetic field or the exchange anisotropy. Therefore, we should give up applying these skillful procedures to $S=1$ random AF spin chain with the anisotropy.

In the present work we therefore adopt the straightforward RSRG procedure and study numerically the renormalization group (RG) flows around the Heisenberg point under staggered magnetic field. The latter very much reduces occurrence of the inadequate renormalization processes, i.e., our present approach is efficient to examine the RG flows against the introduced anisotropy. It is found for the first time that the Heisenberg point, which has a zero average of the exchange coupling anisotropy, is specified as the unstable fixed point against the anisotropy. The result is in disagreement with the previous work by Saguia \textit{et al.}\textsuperscript{12} They studied almost the same model as we do, but without the staggered magnetic field, and concluded that the fixed point situates on the point with a finite average of the exchange anisotropy. A possible origin of the discrepancy is, we consider, the adequacy of the region where the decimation procedures have been executed.

The construction of this paper is as follows. In §2, we introduce our model Hamiltonian. In §3, we briefly show the RSRG method for our Hamiltonian and discuss the confidence of our numerical method. In §4, the numerical results are presented, and in §5 we give the summary of our analysis.

\section{Model}

Our Hamiltonian for the strongly coupled pair of spins $S_1, S_2$ is given by

$$H_0 = JS_1 \cdot S_2 + LS_1^z S_2^z$$
\[-D_1(S_z^1)^2 - D_2(S_z^2)^2 - h_1 S_z^1 - h_2 S_z^2.\] (1)

These spins are weakly coupled to the neighbors via

\[\mathcal{H} = K_1 S_1 \cdot S_1' + K_2 S_2 \cdot S_2' + M_1 S_z^1 S_{t_z}^1 + M_2 S_z^2 S_{t_z}^2\]
\[-D_3(S_{t_z}^1)^2 - D_4(S_{t_z}^2)^2 - h_3 S_z^1 - h_4 S_z^2\]
\[\equiv \mathcal{H} - D_3(S_{t_z}^1)^2 - D_4(S_{t_z}^2)^2 - h_3 S_z^1 - h_4 S_z^2.\] (2)

Diagonalizing \(H_0\), we obtain its eigen values, \(\{E_k \mid k = 0, 1, \ldots, 8\}\), with their eigen states, \(\{|k\} \mid k = 0, 1, \ldots, 8\}\), where we take \(|0\rangle\) as the two-spins ground state. As long as the magnetic field is staggered, i.e., \(h_1 h_2 \leq 0\), \(|0\rangle\) is always non-degenerated. Introducing the magnetic field, we should have both the uniform anisotropy \(L\) and the uniaxial anisotropy \(D\) even when we start the renormalization process from the state with all \(L_{ij} = 0\) and \(D_i = 0\).

§3. Real-Space Renormalization Group Method

In the present work we restrict our consideration to at \(T = 0\). Taking into account \(\mathcal{H}\) by the perturbation expansion and dropping \(O(\mathcal{H}^3)\) terms, we can obtain the modified ground-state energy as

\[E_0 + \langle 0|\mathcal{H}|0\rangle + \sum_{k=1}^{8} \frac{\langle 0|\mathcal{H}|k\rangle^2}{E_0 - E_k}\]
\[= E' + J'S_1' \cdot S_2' + L'S_z^1 S_z^2\]
\[-D'_1(S_{t_z}^1)^2 - D'_2(S_{t_z}^2)^2 - h'_1 S_z^1 - h'_2 S_z^2.\] (3)

The all non-zero matrix elements of

\[\langle 0|\mathcal{H}|k\rangle \equiv \langle 0|\mathcal{H}'|k\rangle\]
\[-[D_3(S_{t_z}^1)^2 + D_4(S_{t_z}^2)^2 + h_3 S_z^1 + h_4 S_z^2]\delta_{0k},\]
\[k = 0, 1, \ldots, 8,\] (4)
in eq. (3) should be required. After some algebra, we obtain the all recursion relations of these renormalized parameters as summerized in Appendix.

Unfortunately, our recursion equations are so complicated that it would be difficult to be solved even in approximated forms. Therefore, we execute the decimation process numerically after our predecessors (see Fig. 1).\(^{11-14}\) Considering a simple case only with isotropic exchange couplings, we can easily find that this perturbative renormalization group for \(S \geq 1\) chain is not adequate.\(^{11,14}\)

In fact, we obtain the recursion relation for the isotropic exchange coupling of a spin-S chain as

\[J' = \frac{2S(S + 1) K_1 K_2}{3J}\] (5)

within \(O(\mathcal{H}^2)\), and this coefficient \(2S(S+1)/3\) is larger than unity for \(S \geq 1\). However, only in the strongly disordered limit with staggered field, the singlet-triplet energy-level differences are typically
so larger than the nearest neighbor couplings that we can rarely find the inadequate decimation processes, in which \( J' > J \). Actually in our numerical analysis such inadequate decimation processes occur within 3\% to the whole decimation processes. We should take into account that our numerical results contain the intrinsic errors within 3\%, and point out that our numerical conclusion is obtained within this accuracy.

In the present work we analyze systems in the strongly disordered limit, i.e., the initial distribution of exchange couplings \( \{ J_{i,j} \} \) is chosen as \( P(0 \leq J_{i,j} \leq 1) = 1 \). We introduce the random staggered field with the distribution as \( P(0 \leq h^A_i \leq h^{max}) = 1/h^{max} \) and \( P(-h^{max} \leq h^B_i \leq 0) = 1/h^{max} \), where \( h^{max} \) is varied, and \( A \) and \( B \) mean sub-lattices’ indexes. Decimating until the maximum of \( J_{ij} \) becomes less then the cutoff energy \( \Omega \), a parameter which specifies the degree of decimation, we obtain averages of the renormalized parameters corresponding to \( \Omega \). In order to obtain the reliable results, we should check that \( J_{ij} \) is the largest energy-scale among those involved in the problem such as \( |L_{ij}|, |D_i|, \) and \( |h_i| \), in each renormalization step. If, for example, we start our decimation step from the point with \( \langle \delta \rangle > 0 \), where \( \delta \equiv L_{ij}/J_{ij} \) and \( \langle \cdots \rangle \) denotes the average over the remaining bonds in each decimation step, already for \( \Omega \sim 0.3 \) we are faced to the case with \( \delta \sim 1 \) (see Fig. 3 below), where our RG rule cannot work well. For \( \langle \delta \rangle < -0.2 \), on the other hand, it turns out that inadequate processes occur more than 3\%. Therefore, we should restrict our quantitative analyses within only decimation steps for which \( \Omega \) stays a few tenths of maximum of initial \( J_{ij} \). For this purpose, we need to prepare such a large system that the averaged values can be obtained within small errors even if \( \Omega \) stays in such a large value. Our system initially contains \( 2^{15} = 32768 \) spins, and the number of samples examined is 100. We call the isotropic point with both \( \langle \delta \rangle = 0 \) and \( \langle \bar{h} \rangle = 0 \) the Heisenberg point, where \( |\langle \bar{h} \rangle| \equiv |\langle h^A \rangle| + |\langle h^B \rangle| \).

§4. Results

In Fig. 2, we show a typical RG flow in the \( |\langle \bar{h} \rangle| - \langle \delta \rangle \) plain. As seen in the figure, the staggered field is an irrelevant perturbation on the line, where \( \langle \delta \rangle = 0 \). We can also show that RG flows accumulate on the Heisenberg point along this line as far as \( 0 < |\langle \bar{h} \rangle| \ll \Omega \).

Taking the initial value of \( \langle \bar{h} \rangle \) as 0 strictly, we could only obtain uncertain results on the flows.
near the Heisenberg point because the RG flows are intrinsically unstable. However, setting small but finite values of $\langle \tilde{h} \rangle$ first, we can observe the systematic RG flows near the Heisenberg point as shown in Fig.3. In the figure, we show the RG flows under decreasing $\Omega$ from the initial points with $|\langle \tilde{h} \rangle| = 0.0004$ and $\langle \delta \rangle \neq 0$. The situations are completely different between $\langle \delta \rangle > 0$ and $\langle \delta \rangle < 0$. The RG flows approach toward the point $\langle \delta \rangle = -1$ in the area $\langle \delta \rangle < 0$, while they become the infinity as $\langle \delta \rangle \rightarrow \infty$ in the area $\langle \delta \rangle > 0$. These two fixed points, $\langle \delta \rangle = -1$ and $\langle \delta \rangle \rightarrow \infty$ have been called the XX RS and ZAF point, respectively, and they correspond to the different phases.

We can also confirm that the averaged single-ion anisotropy, $\langle D \rangle$, behaves differently between in the XX RS and in the ZAF phases. In the XX RS phase, $\langle D \rangle < 0$, i.e., preferable to the low-spin state, and their absolute values are comparable to the cutoff energy $\Omega$. On the other hand, in the ZAF phase, $\langle D \rangle > 0$, i.e., preferable to the high-spin state, and their absolute values evolve toward infinity as $\Omega$ being decreased. All these RG flows branch off at the line $\langle \delta \rangle = 0$. According to our more detailed analysis, no critical line can be found more than $\langle \delta \rangle = 0.000(3)$.

Putting together our results discussed so far, we propose the schematic RG flow diagram in the strongly disordered limit as shown in Fig. 4, in which one sees the Heisenberg point is the unstable fixed point. Any definite informations about the feature of the Heisenberg point cannot be obtained due to the intrinsic numerical difficulties in our formalism. However, referring to the results by other methods, $^{3-5, 10}$ we can identify this unstable fixed point as the XXX RS point. The feature of the Heisenberg point should be qualitatively the same as the Heisenberg point of the $S=\frac{1}{2}$ chain. $^8$
§5. Summary

We have analyzed the strongly disordered S=1 AF quantum spin chain by the numerical RSRG method. The RG flows around the Heisenberg point $\langle \delta \rangle = 0$ can be investigated by introducing the small staggered field, which is the irrelevant perturbation for our renormalization process. We have carefully executed numerical decimation processes in such a way that few inadequate processes are involved. Consequently, we have obtained the reliable RG flows around the Heisenberg point within
the sufficient accuracy. It is concluded that the Heisenberg point is the unstable fixed point against anisotropy, and that it turns from(to) XX RS phase to(from) ZAF phase due to infinitesimal changes of anisotropic couplings.

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Appendix: Recursion Relations

The recursion relations for the renormalized parameters in eq. (3) are described as:

\[ E' = E_0 - 2 \left[ \frac{(A_3)^2 + (B_3)^2}{E_3 - E_0} + \frac{(A_4)^2 + (B_4)^2}{E_4 - E_0} + \frac{(A_5)^2 + (B_5)^2}{E_5 - E_0} + \frac{(A_6)^2 + (B_6)^2}{E_6 - E_0} \right], \]

\[ J' = 2 \left[ -\frac{A_3B_3}{E_3 - E_0} - \frac{A_4B_4}{E_4 - E_0} - \frac{A_5B_5}{E_5 - E_0} - \frac{A_6B_6}{E_6 - E_0} \right], \]

\[ L' = 2 \left[ -\frac{A_1B_1}{E_1 - E_0} - \frac{A_2B_2}{E_2 - E_0} \right] - J', \]

\[ D'_1 = D_3 + \frac{(A_1)^2}{E_1 - E_0} + \frac{(A_2)^2}{E_2 - E_0} - \frac{(A_3)^2}{E_3 - E_0} - \frac{(A_4)^2}{E_4 - E_0} - \frac{(A_5)^2}{E_5 - E_0} - \frac{(A_6)^2}{E_6 - E_0}, \]

\[ D'_2 = D_4 + \frac{(B_1)^2}{E_1 - E_0} + \frac{(B_2)^2}{E_2 - E_0} - \frac{(B_3)^2}{E_3 - E_0} - \frac{(B_4)^2}{E_4 - E_0} - \frac{(B_5)^2}{E_5 - E_0} - \frac{(B_6)^2}{E_6 - E_0}, \]

\[ h'_1 = h_3 - A_0 - \frac{1}{2} \left[ \frac{(A_3)^2}{E_3 - E_0} + \frac{(A_4)^2}{E_4 - E_0} - \frac{(A_5)^2}{E_5 - E_0} - \frac{(A_6)^2}{E_6 - E_0} \right], \]

\[ h'_2 = h_3 - B_0 - \frac{1}{2} \left[ \frac{(B_3)^2}{E_3 - E_0} + \frac{(B_4)^2}{E_4 - E_0} - \frac{(B_5)^2}{E_5 - E_0} - \frac{(B_6)^2}{E_6 - E_0} \right]. \] (A.1)

Hereafter, we use the abbreviations, \( \bar{L} \equiv L + D_1 + D_2 \), \( \bar{h} \equiv h_1 - h_2 \), \( h_1^\pm \equiv h_1 \pm D_1 \), and \( h_2^\pm \equiv h_2 \pm D_2 \). In eqs.(A.1), \( E_0 \), \( E_1 \), and \( E_2 \) should be represented differently, whether \( \bar{h} = 0 \) or not. When \( \bar{h} = 0 \),

\[ E_0 = -\frac{1}{2} \left[ \sqrt{(J + \bar{L})^2 + 8J^2} + \bar{J} + \bar{L} \right], \]

\[ E_1 = \bar{J} - \bar{L}, \]

\[ E_2 = \frac{1}{2} \left[ \sqrt{(J + \bar{L})^2 + 8J^2} - \bar{J} - \bar{L} \right]. \] (A.2)

When \( \bar{h} \neq 0 \),

\[ E_n = \frac{2}{3} \left[ p \cos \left( \frac{1}{3} \left\{ \arccos \left[ p^{-3}(J + \bar{L}) \left\{ (J + \bar{L})^2 + 9J^2 - 9\bar{h}^2 \right\} + 2\pi(n + 1) \right] \right\} \right) - J - \bar{L} \], \]

\[ p = \left[ (J + \bar{L})^2 + 6J^2 + 3\bar{h}^2 \right]^{1/2}, \quad n = 0, 1, 2. \] (A.3)
On the other hand, $E_3, E_4, E_5$, and $E_6$ can be described independently of $\bar{h}$:

$$ E_3 = \frac{1}{2}(h_1^- + h_2^- - x^-), $$
$$ E_4 = \frac{1}{2}(h_1^- + h_2^- + x^-), $$
$$ E_5 = \frac{1}{2}(-h_1^+ - h_2^+ - x^+), $$
$$ E_6 = \frac{1}{2}(-h_1^+ - h_2^+ + x^+), $$

(A.4)

using the abbreviation $x^\pm = [4J^2 + (h_1^\pm - h_2^\pm)^2]^{1/2}$. $A_k$ and $B_k$ also depends on $\bar{h}$.

When $\bar{h} = 0$,

$$ A_0 = B_0 = A_2 = B_2 = 0, $$
$$ A_1 = \sqrt{2}J(K_1 + M_1)r_0^{-1}, $$
$$ B_1 = -\sqrt{2}J(K_2 + M_2)r_0^{-1}, $$
$$ A_3 = [2J^2 - (E_0 + J + \bar{L})(h_1^- - h_2^- + x^-)k_1(\sqrt{2}r_0r_3)^{-1}, $$
$$ B_3 = [2(J_0 + J + \bar{L})(h_1^- - h_2^- + x^-)K_2(\sqrt{2}r_0r_3)^{-1}, $$
$$ A_4 = [2J^2 - (E_0 + J + \bar{L})(h_1^- - h_2^- - x^-)K_1(\sqrt{2}r_0r_4)^{-1}, $$
$$ B_4 = [2(J_0 + J + \bar{L})(h_1^- - h_2^- - x^-)K_2(\sqrt{2}r_0r_4)^{-1}, $$
$$ A_5 = [2J^2 + (E_0 + J + \bar{L})(h_1^- - h_2^- - x^-)K_1(\sqrt{2}r_0r_5)^{-1}, $$
$$ B_5 = [2J^2 + (E_0 + J + \bar{L})(h_1^- - h_2^- - x^-)K_2(\sqrt{2}r_0r_5)^{-1}, $$
$$ A_6 = [2J^2 + (E_0 + J + \bar{L})(h_1^- + h_2^- + x^-)K_1(\sqrt{2}r_0r_6)^{-1}, $$
$$ B_6 = [2J^2 + (E_0 + J + \bar{L})(h_1^- + h_2^- + x^-)K_2(\sqrt{2}r_0r_6)^{-1}, $$

$$ r_0 = [(E_0 + J + \bar{L})^2 + 2J^2]^{1/2}. $$

(A.5)

And when $\bar{h} \neq 0$,

$$ A_0 = -4\tilde{h}J^2(E_0 + J + \bar{L})(K_1 + M_1)r_0^{-2}, $$
$$ B_0 = 4\tilde{h}J^2(E_0 + J + \bar{L})(K_2 + M_2)r_0^{-2}, $$
$$ A_1 = -2\tilde{h}J^2(E_0 + E_1 + 2J + 2\bar{L})(K_1 + M_1)(r_0r_1)^{-1}, $$
$$ B_1 = 2\tilde{h}J^2(E_0 + E_1 + 2J + 2\bar{L})(K_2 + M_2)(r_0r_1)^{-1}, $$
$$ A_2 = -2\tilde{h}J^2(E_0 + E_2 + 2J + 2\bar{L})(K_1 + M_1)(r_0r_2)^{-1}, $$
$$ B_2 = 2\tilde{h}J^2(E_0 + E_2 + 2J + 2\bar{L})(K_2 + M_2)(r_0r_2)^{-1}, $$
$$ A_3 = (E_0 + J + \bar{L} - \bar{h})[2J^2 - (E_0 + J + \bar{L} + \bar{h})(h_1^- - h_2^- + x^-)K_1(\sqrt{2}r_0r_3)^{-1}, $$
$$ B_3 = (E_0 + J + \bar{L} + \bar{h})[2(J_0 + J + \bar{L} - \bar{h})(h_1^- - h_2^- + x^-)K_2(\sqrt{2}r_0r_3)^{-1}, $$
$$ A_4 = (E_0 + J + \bar{L} - \bar{h})[2J^2 - (E_0 + J + \bar{L} + \bar{h})(h_1^- - h_2^- - x^-)K_1(\sqrt{2}r_0r_4)^{-1}, $$

(A.6)
\[ B_4 = (E_0 + J + \tilde{L} + \tilde{h})[2(E_0 + J + \tilde{L} - \tilde{h}) - (h_1^+ - h_2^- - x^-)]JK_2(\sqrt{2}r_0r_4)^{-1}, \]
\[ A_5 = (E_0 + J + \tilde{L} + \tilde{h})[2(E_0 + J + \tilde{L} - \tilde{h}) + h_1^+ - h_2^- - x^+]JK_2(\sqrt{2}r_0r_5)^{-1}, \]
\[ B_5 = (E_0 + J + \tilde{L} - \tilde{h})[2J^2 + (E_0 + J + \tilde{L} + \tilde{h})(h_1^+ - h_2^- - x^+)]JK_2(\sqrt{2}r_0r_5)^{-1}, \]
\[ A_6 = (E_0 + J + \tilde{L} + \tilde{h})[2(E_0 + J + \tilde{L} - \tilde{h}) + h_1^+ - h_2^- + x^+]JK_2(\sqrt{2}r_0r_5)^{-1}, \]
\[ B_6 = (E_0 + J + \tilde{L} - \tilde{h})[2J^2 + (E_0 + J + \tilde{L} + \tilde{h})(h_1^+ - h_2^- + x^+)]JK_2(\sqrt{2}r_0r_5)^{-1}, \]
\[ r_n = [(E_n + J + \tilde{L})^2 - \tilde{h}^2]^1/2 + 2((E_n + J + \tilde{L}) + \tilde{h})^2J^2]^{1/2}, \quad n = 0, 1, 2. \tag{A.6} \]

In eqs.\(\text{(A.5)}\) and\(\text{(A.6)}\), \(r_3, r_4, r_5, \) and \(r_6\) are common:

\[ r_3 = [2x^-(x^- + h_1^- - h_2^-)]^{1/2}, \]
\[ r_4 = [2x^-(x^- - h_1^- + h_2^-)]^{1/2}, \]
\[ r_5 = [2x^+(x^+ - h_1^+ + h_2^+)]^{1/2}, \]
\[ r_6 = [2x^+(x^+ + h_1^+ - h_2^+)]^{1/2}. \tag{A.7} \]

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