Field-Induced Multiple Reentrant Quantum Phase Transitions in Randomly Dimerized Antiferromagnetic $S = 1/2$ Heisenberg Chains

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The multiple reentrant quantum phase transitions in the $S = 1/2$ antiferromagnetic Heisenberg chains with random bond alternation in the magnetic field are investigated by the density matrix renormalization group method combined with interchain mean field approximation. It is assumed that odd numbered bonds are antiferromagnetic with strength J and even numbered bonds can take the values $J_{\rm S}$ and $J_{\rm W}$ ($J_{\rm S} > J > J_{\rm W} > 0$) randomly with the probabilities p and $1-p$, respectively. The pure version ($p = 0$ and $p = 1$) of this model has a spin gap but exhibits a field-induced antiferromagnetism in the presence of interchain coupling if Zeeman energy due to the magnetic field exceeds the spin gap. For $0 < p < 1$, antiferromagnetism is induced by randomness at the small field region where the ground state is disordered due to the spin gap in the pure version. At the same time, this model exhibits randomness-induced plateaus at several values of magnetization. The antiferromagnetism is destroyed on the plateaus. As a consequence, we find a series of reentrant quantum phase transitions between transverse antiferromagnetic phases and disordered plateau phases with the increase of magnetic field for a moderate strength of interchain coupling. Above the main plateaus, the magnetization curve consists of a series of small plateaus and jumps between them. It is also found that antiferromagnetism is induced by infinitesimal interchain coupling at the jumps between the small plateaus. We conclude that this antiferromagnetism is supported by the mixing of low-lying excited states by the staggered interchain mean field even though the spin correlation function is short ranged in the ground state of each chain.

KEYWORDS: random quantum spin chain, DMRG, disorder-induced order, field-induced order, randomness-induced plateau, reentrant phase transition

1. Introduction

In recent studies of one-dimensional quantum spin systems, exotic quantum phases induced by a strong magnetic field have been attracting broad interest. Among them, field-induced transverse antiferomagnetism has been widely investigated in many experimental and theoretical studies.[1–4] If a magnetic field larger than the spin gap is applied to a spin-gapped system, the single-chain ground state becomes the Tomonaga-Luttinger liquid and the transverse antiferromagnetic order develops as soon as a weak interchain coupling is switched on.

Disorder is another origin of order in spin-gapped low dimensional quantum magnets.[5–11] In the presence of disorder, spins in the nonmagnetic ground state revive and induce so-called 'disorder-induced order' even in the absence of magnetic field.

On the other hand, the possibility of a disorder-induced magnetization plateau is also predicted in a certain class of one-dimensional random quantum magnets.[11–16] This corresponds to the spin gap state induced by disorder and magnetic field.

Therefore, the effect of disorder on quantum magnets in a magnetic field is twofold. Namely, disorder enhances magnetic order by reviving spins, while it suppresses magnetic order by forming plateaus. In the present work, we investigate the competition between these two contradictory aspects of randomness in quasi-one-dimensional quantum spin systems and the resulting multiple reentrant phase transitions between transverse antiferromagnetic phases and disordered plateau phases. Similar problem has been discussed by Mikeska *eat al.*[14] for the diluted dimer network system and by Nohadani *et al.*[15,16] for the coupled random dimer network.

This paper is organized as follows. In the next section, the model Hamiltonian is presented. The single-chain magnetization curve is calculated in §3. Within the interchain mean field approximation, we predict the multiple reentrant behavior with the increase in magnetic field in §4. The calculation of the spin-spin correlation function is presented in §5. Even in the non-plateau state, where infinitesimal interchain coupling induces transverse ordering, the correlation function of a single chain turned out to be short ranged. On the basis of these observations, the mechanism of antiferromagnetism away from the plateau region is explained in §5. The final section is devoted to summary and discussion.

2. Model Hamiltonian

As a candidate model in which reentrant antiferromagnetism is expected, we investigate the quasi-one-dimensional random dimerized $S = 1/2$ Heisenberg chain whose Hamiltonian is given by

$$\mathcal{H} = \sum_j \left\{ \sum_{i=1}^{N/2} J\boldsymbol{S}_{2i-1,j}\boldsymbol{S}_{2i,j} + \sum_{i=1}^{N/2} J_{ij}\boldsymbol{S}_{2i,j}\boldsymbol{S}_{2i+1,j} \right\}$$

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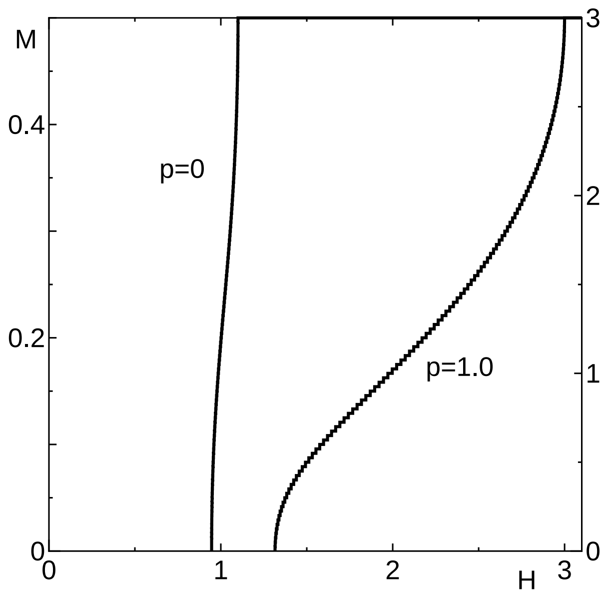

Fig. 1. Magnetization curves of pure single chains with p=0 and 1.0. The chain length is $N = 240$.

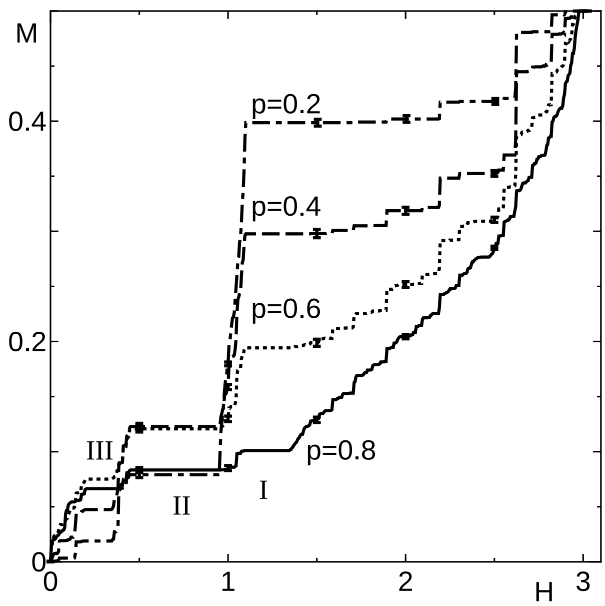

Fig. 2. Magnetization curve of single chains for p=0.2, 0.4, 0.6 and 0.8. The chain length is $N = 120$. Magnetization is measured for the middle 60 sites to reduce the boundary effect. The average is taken over 64 samples. Error bars are shown only for selected points because otherwise the symbols are extremely dense.

$$+ \sum_{i=1}^{N} \sum_{<j,j'>} J_{\rm int} \boldsymbol{S}_{i,j} \boldsymbol{S}_{i,j'}, \qquad (1)$$

where $J_{ij} = J_{\rm S}$ with the probability p and $J_{ij} = J_{\rm W}$ with the probability $1-p$. The interchain exchange coupling is denoted by $J_{\rm int}$. The spin operator $\boldsymbol{S}_{i,j}$ denotes the spin on the i-th site of the j-th chain. The summation $\sum_{<j,j'>}$ is taken over all nearest neighbour pairs of chains. In the present work, we assume $J_{\rm S} > J > J_{\rm W} > 0$. A similar model with ferromagnetic $J_{\rm W}$ has been discussed[11] in relation to experimental materials.[5]

3. Single-Chain Magnetization Curve

The ground state magnetization curve of a single chain with $J_{\rm int} = 0$ in (1) is calculated using the density matrix renormalization group (DMRG) method. The magnetization per site M is defined by

$$M \equiv \frac{1}{N} \sum_{i=1}^{N} \langle S_i^z \rangle, \qquad (2)$$

where the summation is taken over all spins in a single chain and the chain index j is suppressed. Regular models with $p = 0$ or $p = 1$ have magnetization plateaus at $M = 0$, which corresponds to the spin gap and at the saturation magnetization $M = M_{\rm s} \equiv 1/2$. However, they have no plateaus with intermediate values of magnetization as shown in Fig. 1.

On the other hand, the magnetization curves for $p \neq 0, 1$ consist of a sequence of plateaus. Between them, magnetization increases almost continuously. A typical example is shown in Fig. 2 for $J_{\rm S} = 2, J_{\rm W} = 0.1$ and $J = 1$ for various values of p.

The main features of the magnetization curves can be understood using the cluster picture similar to that described in ref. 11. With the increase in magnetic field, we observe three large plateaus that are numbered I, II and III in Fig. 2. Let us consider a cluster consisting of q successive $J_{\rm S}$-bonds and $q-1$ J-bonds in between. This is called the 'q-cluster' as in ref. 11. The $2q$ spins in a cluster form a strongly coupled singlet cluster. The two spins connected to both ends of this cluster by J-bonds are almost free but weakly coupled mediated by the quantum fluctuation within the strongly coupled cluster. Other spins form singlet dimers on the J-bonds if $J_{\rm W} << J$.

On plateau I with magnetization $M = (1-p)M_{\rm s}$, spins that do not belong to the q-clusters are all polarized. On plateau II, end spins separated by 1-clusters with a single $J_{\rm S}$-bond remain unpolarized. Similarly, on plateau III, end spins separated by 2-clusters also remain unpolarized and so on. These interpretations are confirmed by comparing them with the magnetization process of a cluster consisting of a q-cluster and two additional end spins connected by J-bonds on both ends of the q-cluster. Lower plateaus due to spins separated by longer q-clusters are not clearly identified within the present scale. The low field part of the magnetization curve reflects the singularity of the low energy excitation spectrum as described in ref. 11.

Above plateau I, magnetization increases with the series of plateaus and narrow continuous parts up to the saturation field. As p increases, the width of the plateaus decreases and magnetization curve becomes almost continuous.

4. Effect of Interchain Exchange Interaction

We treat interchain coupling by mean field approximation[17] assuming the transverse antiferromagnetic order as

$$\langle S_{i,j}^x \rangle = \begin{cases} (-1)^i m & J_{\rm int} < 0 \\ (-1)^i P_j m & J_{\rm int} > 0. \end{cases} \qquad (3)$$

For $J_{\rm int} > 0$, we assume that the two dimensional lattice of the chains is bipartite. The value of P_j is $+1$ if the site j belongs to one of the sublattices and -1 if it belongs to the other. We thus have the interchain mean field Hamiltonian $H^{\rm IMF}$ for each chain as

$$\mathcal{H}^{\rm IMF} = \sum_{i=1}^{N/2} J\boldsymbol{S}_{2i-1}\boldsymbol{S}_{2i} + \sum_{i=1}^{N/2} J_i\boldsymbol{S}_{2i}\boldsymbol{S}_{2i+1} - H_{\rm st}\sum_{i=1}^{N}(-1)^i S_i^x, \quad (4)$$

with $H_{\rm st} = z|J_{\rm int}|m$. If we denote the staggered magnetization m calculated using given value of $H_{\rm st}$ by $m(H_{\rm st})$, the self-consistent equation reads

$$H_{\rm st} = \lambda m(H_{\rm st}), \quad (\lambda \equiv z|J_{\rm int}|). \quad (5)$$

Therefore, the minimum interchain coupling that stabilizes transverse ordering is given by $\lambda_c = \lim_{H_{\rm st}\to 0} H_{\rm st}/m(H_{\rm st})$, which is equal to the inverse of the single-chain staggered susceptibility $\chi_{\rm st}$. If $\chi_{\rm st}$ diverges, the transverse ordering is stabilized for the infinitesimal interchain coupling within the interchain mean field approximation. Practically, we estimate $m(H_{\rm st})$ numerically with a tiny $H_{\rm st}$ and estimate λ_c from the ratio $H_{\rm st}/m(H_{\rm st})$.

Figure 3 shows the magnetic field dependence of $\lambda_{\rm c}(H_{\rm st})$ estimated with $H_{\rm st} = 0.0005$ for $p = 0.2$ and $p = 0.8$ as representatives of small p and large p cases. The magnetization curves in the absence of staggered field are also presented. The H-$\lambda_{\rm c}(H_{\rm st})$ curve has multiple maxima, which clearly shows that multiple reentrant behavior takes place for finite interchain coupling in the ground state. It should be noted that the H-$\lambda_{\rm c}(H_{\rm st})$ curves are insensitive to the values of $H_{\rm st}$ around these maxima. However, around the dips and minima, the values of $\lambda_{\rm c}(H_{\rm st})$ have significant $H_{\rm st}$-dependence.

For $p = 0.8$, $\lambda_{\rm c}(H_{\rm st})$ remains significantly small above the main plateaus compared with the peak values on the main plateaus. Therefore, we expect no disordered phase for moderate values of interchain coupling in this region where the magnetization curve appears almost continuous. Even away from the main plateaus, however, the magnetization curve shows a series of small plateaus and narrow continuous parts between them. Correspondingly, $\lambda_{\rm c}(H_{\rm st})$ tends to a finite value as $H_{\rm st} \to 0$ on these plateaus. The detailed features of such behavior are shown in Fig. 4 for $2.17 \le H \le 2.21$ as a representative. On these small plateaus, $\lambda_{\rm c}(H_{\rm st})$ clearly tends to small finite values as shown in Fig. 4 around $H = 2.173$ and $H = 2.208$. On the other hand, in the true off-plateau state, $\lambda_{\rm c}(H_{\rm st})$ tends to zero, suggesting the divergence of $\chi_{\rm st}$. In this case, the transverse antiferromagnetic order is stabilized in the presence of infinitesimal interchain interaction. In Fig. 4, such behavior is observed at $H = 2.1905$. To investigate this behavior in more detail, we present the $H_{\rm st}$-dependence of $\lambda_{\rm c}(H_{\rm st})$ in Fig. 5 at $H = 2.1925, 2.1905$ and 2.188 using the data for N =480. Only a 0.2% deviation from $H = 2.1905$ causes a clear upturn of $\lambda_{\rm c}(H_{\rm st})$. Although a weak size dependence is present, the data for $N = 240$ plotted in smaller

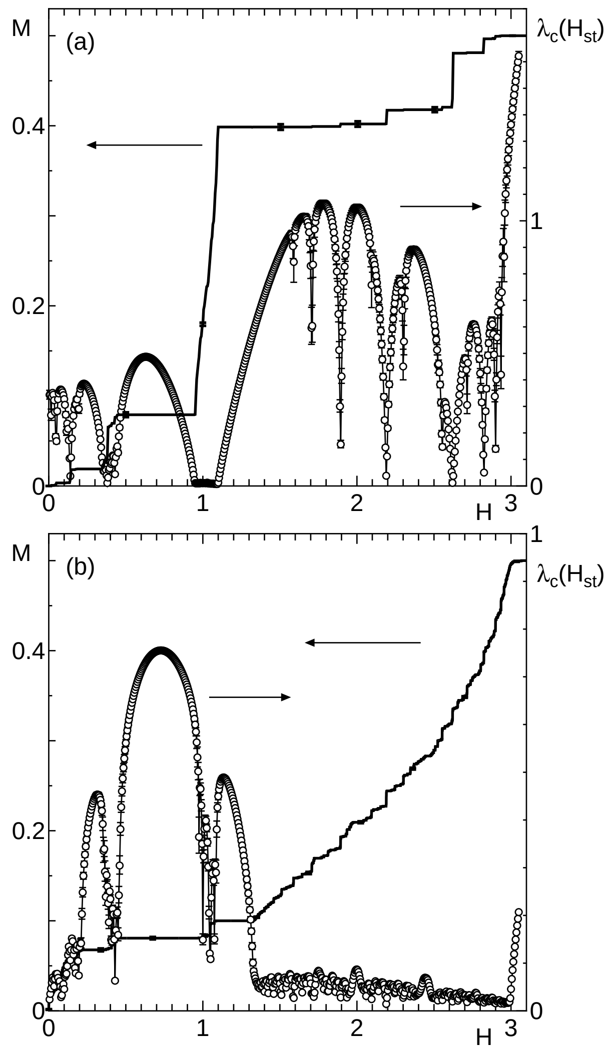

Fig. 3. H-dependence of $\lambda_{\rm c}(H_{\rm st})$ with $H_{\rm st} = 0.0005$ for (a) $p = 0.2$ and (b) $p = 0.8$. The magnetization curves are also shown for reference. The staggered magnetization m is measured for the middle 60 sites to reduce the boundary effect. The chain length is $N = 120$ and the average is taken over 512 samples. Error bars are shown only for selected points.

symbols also show a similar behavior. Therefore, we expect that this is not the finite size effect but is an essential feature of the present system in the thermodynamic limit. A similar behavior is observed for other values of H above the main plateaus. Therefore, we conclude that the antiferromagnetic order is stabilized by infinitesimal interchain coupling only within a narrow region where magnetization increases continously between successive small plateaus.

5. Correlation Functions

To obtain more insight into the nature of each state on the basis of the properties of single chains, we also investigated the spin-spin correlation function $\langle S_i^x S_j^x \rangle$ as a function of $|i-j|$. Figure 6 shows $\left|\langle S_i^x S_j^x \rangle\right| \left(= (-1)^{i-j}\langle S_i^x S_j^x \rangle\right)$ for $H = 2.1905(\circ)$ where $\lambda_{\rm c}$ tends to 0 and $\chi_{\rm st}(H_{\rm st})$ diverges. Even in this case, the spin-spin correlation function is short ranged. Indeed, the behavior of the corelation function is almost the same as

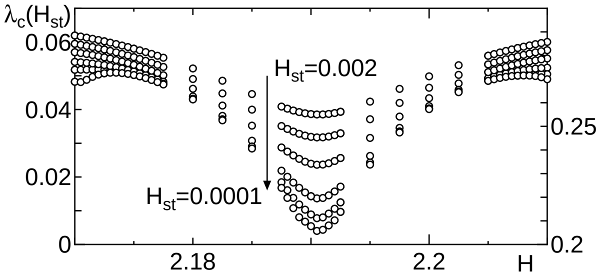

Fig. 4. H-dependence of λ_c for $2.17 \leq H \leq 2.21$. The values of the staggered field are $H_{st} = 0.002, 0.0015, 0.001, 0.0005, 0.00025$ and 0.0001 from top to bottom. The chain length is $N = 480$ and measurement is carried out for the middle 240 sites. The average is taken over 256 samples. The error bars are within the size of the symbols.

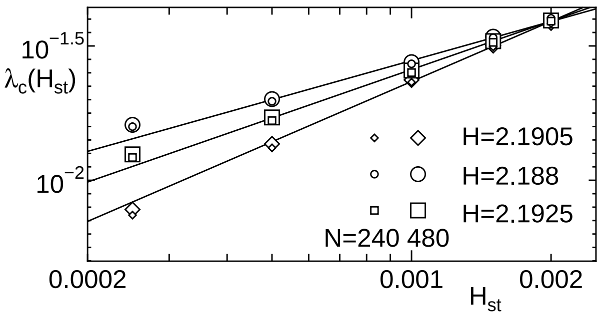

Fig. 5. H_{st}-dependence of λ_c around $H = 2.1905$. The big symbols are for $N = 480$ and the small symbols are for $N = 240$. The solid lines are power law extrapolation from $H_{st} = 0.0005, 0.001, 0.0015$ and 0.002 for $N = 480$. The average is taken over 256 samples.

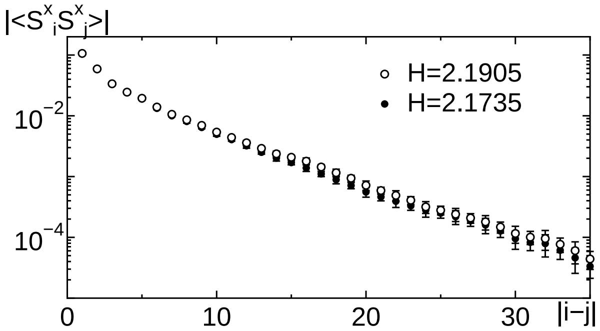

Fig. 6. Transverse correlation function $|\left\langle S_i^x S_j^x \right\rangle|$ at $H = 2.1905(\circ)$ where $\chi_{st}(H_{st} \to 0)$ diverges and at $H = 2.1735(\bullet)$ where $\chi_{st}(H_{st} \to 0)$ is finite. The average is taken over 512 samples for $N = 240$.

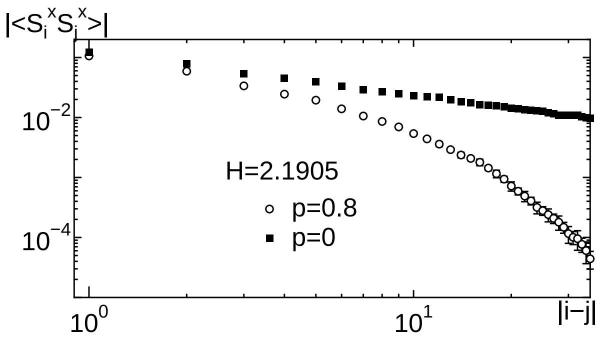

Fig. 7. Log-log plot of correlation function with $p = 0.8$ (open circles) and $p = 1$(filled squares) at $H = 2.1905$ for $N = 240$.

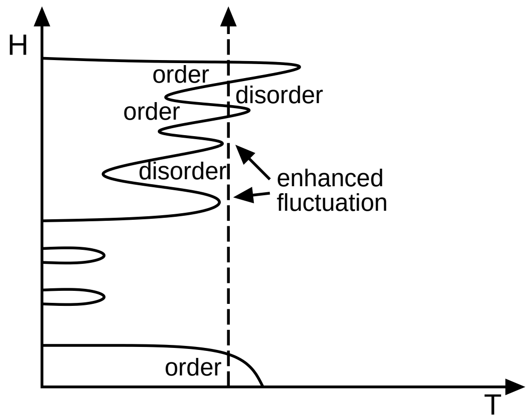

Fig. 8. Schematic finite temperature phase diagram on $H - T$-plane.

that for $H = 2.1735(\bullet)$ where λ_c tends to small but finite values and $\chi_{st}(H_{st})$ tends to large but finite values. In Fig. 7, the log-log plot of the same correlation function is compared with that for the regular chain with $p = 1$ at $H = 2.1905$. It is clear that the rapid decay of correlation for the random chain is distinct from the power law decay for the regular chain.

This can be understood as follows. In the off-plateau region, the continuum of low energy excited states pile up on the ground state. In many of these excited states, the spins that are not correlated in the ground state are correlated. The staggered transverse magnetic field mixes up these excited states resulting in divergent staggered susceptibility. In this case, the long range transverse order can be stablized by infinitesimal interchain coupling even though the spin correlation is short ranged in the ground state. On the other hand, in the plateau state, there exists no low-energy excited states that support the long range order with small interchain coupling.

It should also be noted that the divergence of χ_{st} does not always contradict finite correlation length, because the staggered magnetization does not commute with the Hamiltonian and the summation $\sum_{i,j}(-1)^{i-j}\left\langle S_i^x S_j^x \right\rangle$ is not directly proportional to χ_{st}.

6. Summary and Discussion

The transverse magnetic ordering in the ground state of the random quantum Heisenberg chain is investigated using the density matrix renormalization group and the interchain mean field approximation. It is predicted that the multiple reentrant behavior takes place between the disordered plateau phases and transverse antiferromagnetic ordered phases. This is in contrast to the case of random dimer networks discussed by Mikeska *et al.*[14] and Nohadani *et al.*,[15,16] in which the reentrant transition takes place only once.

It is also pointed out that even in the non-plateau regime the spin-spin correlation of the single chain is short ranged. Nevertheless, the long range order is established with infinitesimal interchain interaction with the help of excited states that pile up near the ground state and are mixed up by the interchain staggered mean field.

In this work we concentrated on the ground state phase transition. Nevertheless, the reentrant behavior should survive even at finite temperatures. The transition temperature should be high between the plateau region and low or zero on the plateau region as shown in Fig. 8 schematically. This behavior manifests itself as anomalous behavior even above the transition temperature. Therefore, if we increase magnetic field at a fixed temperature, the transverse spin fluctuation would be strongly enhanced when we pass near the ordered phase.

We expect that the present type of reentrant behavior is universal in random quantum spin systems in which singlet dimer formation is randomly perturbed to produce local almost free spins. In contrast to the random dimer network systems in which dilution produces isolated spins, the free spins in the present system are produced by the random competition between two different dimer interactions $J_{\rm S}$ and J, each of which prefers different dimer configuration. This is the origin of a more complicated structure of the phase diagram. Thus, we expect the reentrant behavior due to similar mechanism in a variety of systems.

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