

Effect of geometrical frustration on inverse freezingM. Schmidt,^{1,*} C. V. Morais,² and F. M. Zimmer^{1,†}¹*Departamento de Física, Universidade Federal de Santa Maria, 97105-900, Santa Maria, RS, Brazil*²*Instituto de Física e Matemática, Universidade Federal de Pelotas, 96010-900 Pelotas, RS, Brazil*

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The interplay between geometrical frustration (GF) and inverse freezing (IF) is studied within a cluster approach. The model considers first-neighbor (J_1) and second-neighbor (J_2) intracluster antiferromagnetic interactions between Ising spins on a checkerboard lattice and long-range disordered couplings (J) among clusters. We obtain phase diagrams of temperature versus J_1/J in two cases: the absence of J_2 interaction and the isotropic limit $J_2 = J_1$, where GF takes place. An IF reentrant transition from the spin-glass (SG) to paramagnetic (PM) phase is found for a certain range of J_1/J in both cases. The J_1 interaction leads to a SG state with high entropy at the same time that can introduce a low-entropy PM phase. In addition, it is observed that the cluster size plays an important role. The GF increases the PM phase entropy, but larger clusters can give an entropic advantage for the SG phase that favors IF. Therefore, our results suggest that disordered systems with antiferromagnetic clusters can exhibit an IF transition even in the presence of GF.

DOI: [10.1103/PhysRevE.93.012147](https://doi.org/10.1103/PhysRevE.93.012147)**I. INTRODUCTION**

Inverse transitions are interesting and unusual phenomena that have received considerable attention recently. In such transformations, the more ordered phase is cooled down into a disordered one. In systems that present inverse transition, a subtle balance between energy and entropy can be pointed to as a fundamental aspect [1,2]. To shed some light on the key physical elements of this balance, magnetic models have been used extensively. For instance, mechanisms able to affect the entropic behavior of phases under consideration can be relevant to understand possible routes to inverse transitions. It is known that geometrical frustration (GF) affects strongly the entropy of magnetic systems [3]. Therefore, GF could be an important element to consider in the inverse transition study, but few efforts have been made in this direction. This specific point motivates the present work, in which the interplay between inverse transitions and GF is the main subject.

Spin-1 models have been prototypes to study inverse transitions. For example, Schupper and Shnerb have proposed that inverse transitions could appear in the Blume-Capel model when the relation between the degeneracy of the interacting ($S^z = \pm 1$) and noninteracting ($S^z = 0$) states is tuned [1,2]. In this case, the noninteracting states are energetically favored by the crystal field D , and the relative degeneracy provides an entropic advantage to the interacting states. When disordered spin-1 models are adopted, an inverse transition from the spin-glass (SG) state to the paramagnetic (PM) phase, called inverse freezing (IF), can be found. Interestingly, the IF occurs without requiring this artificial entropic advantage, as shown by Monte Carlo simulations [4,5], mean-field theory [6–9], finite connectivity calculations [10], and a scale-free network [11]. It has been claimed that the presence of frustration caused by disorder can introduce an entropic scenario that supports the IF [1,2,4–6]. In addition, disordered fermionic models can also exhibit IF spontaneously for a certain range of the chemical

potential μ [12,13]. It is important to remark that the previous disordered models follow the Sherrington-Kirkpatrick (SK) type of interaction, where the replica method is used [14]. This leads to precise thermodynamic quantities within the ordered SG phase only in the full replica-symmetry-breaking scheme [6]. As an alternative, the van Hemmen SG model in a fermionic formulation was proposed. This approach avoids the replica technique and can also lead to the IF [15].

Recently, some Ising spin models have been adopted to study inverse transitions [16–20]. For instance, IF was found in a disordered Ising SG model within a cluster approach [19]. The authors consider Ising spin clusters with AF intracluster interactions and the infinite-range SK type of coupling between clusters. Intercluster disorder is strongly dependent on the cluster magnetic moment, and it introduces frustration. Additionally, the AF interactions favor energetically compensated clusters, which are against the intercluster disorder. In this sense, the presence of AF intracluster interactions plays a similar role to the crystal field in spin-1 models, while the frustration coming from disorder introduces the complex entropic scenario to the IF occurrence. Quite recently, this cluster formulation was considered to study the effect of GF in the SG stabilization by adopting the J_1 - J_2 model for intracluster interactions [21]. As a result, the SG phase appears at a lower strength of disorder, and the IF disappears as the GF increases. In Ref. [21], GF supports uncompensated clusters and introduces a high-entropy PM phase at low temperatures. However, the energetic favoring of uncompensated clusters could be enough to undermine the reentrance associated with the IF [19]. Therefore, it raises the following questions: (i) Is the IF still eliminated when fully compensated moments are energetically favored in geometrically frustrated clusters? (ii) How is the entropic behavior of the PM and SG phases changed by GF mainly close to the phase boundary?

Motivated by these issues, we investigate the effect of GF on the IF. We consider the checkerboard lattice divided into clusters. The model allows AF intracluster interactions between first neighbors (J_1) and second neighbors (J_2), with intercluster couplings following a van Hemmen disorder [22,23]. This type of disorder, even lacking the multiplicity of metastable states

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found in the SK model, still retains important fingerprints of spin glasses, such as the behavior of the susceptibility and the specific heat as a function of temperature [22]. It is important to remark that this intercluster disorder can be evaluated without the replica technique leading to an effective single-cluster problem solved by exact diagonalization. This means that the thermodynamic properties within the SG phase, including the entropy, can be obtained without mathematical difficulties related to the replica, which is the main reason for using the van Hemmen disorder in the present study. In addition, the intracluster interactions can introduce two regimes: an AF cluster without GF in the absence of the J_2 interactions, and the geometrically frustrated case in which $J_2 = J_1$. We study this problem for several cluster sizes ($4 \leq n_s \leq 20$), in which the cluster shapes always favor a fully compensated moment in the two regimes of intracluster interactions. Therefore, the entropy change caused by GF in the context of the IF is addressed in the present work.

The paper is organized as follows. In Sec. II, we present the analytical calculation for the disordered cluster approach in the checkerboard lattice. In Sec. III, we investigate the IF by considering phase diagrams, entropic behavior, and intracluster spin-spin correlations. In particular, the interplay between GF and IF is analyzed in Sec. III B. The final section is devoted to the conclusion.

II. MODEL

We consider a checkerboard lattice divided into N_{cl} clusters with n_s spins, which is described by the Hamiltonian

$$H = - \sum_{\nu} \sum_{i,j}^{n_s} J_{ij} \sigma_{\nu_i} \sigma_{\nu_j} - \sum_{\nu,\lambda} \sum_{i,j}^{n_s} J^{\nu\lambda} \sigma_{\nu_i} \sigma_{\lambda_j}, \quad (1)$$

where $\sigma_{\nu_i} = \pm 1$ is the Ising spin of site i of cluster ν . The first term of Eq. (1) corresponds to intracluster interactions. The second term is a van-Hemmen-like infinite-range disordered interaction between clusters given by $J^{\nu\lambda} = \frac{J}{N_{\text{cl}} n_s} (\xi_{\nu} \eta_{\lambda} + \xi_{\lambda} \eta_{\nu})$, where ξ_{ν} 's and η_{λ} 's are independent random variables that follow identical Gaussian distributions with variance 1 [22,24,25]. We can rewrite Eq. (1) as

$$H = \sum_{\nu} H_{J_1-J_2}^{\nu} - \sum_{\nu,\lambda} \frac{J}{N_{\text{cl}} n_s} (\xi_{\nu} \eta_{\lambda} + \xi_{\lambda} \eta_{\nu}) S_{\nu} S_{\lambda}, \quad (2)$$

where $S_{\nu} = \sum_{i=1}^{n_s} \sigma_{\nu_i}$ is the total magnetic moment of the cluster ν , and

$$H_{J_1-J_2}^{\nu} = J_1 \sum_{(i,j)}^{n_s} \sigma_{\nu_i} \sigma_{\nu_j} + J_2 \sum_{\langle i,j \rangle}^{n_s} \sigma_{\nu_i} \sigma_{\nu_j} \quad (3)$$

refers to the AF intracluster interactions, where (i,j) (or $\langle i,j \rangle$) denotes the sum over first-neighbor (or second-neighbor) spins in a given cluster.

The intercluster disorder is evaluated within a usual mean-field treatment, which allows us to express the last term of Eq. (2) in a separable form with quadratic terms. Hubbard-Stratonovich transformations are used to linearize the quadratic terms by introducing fields $q_1(\xi, \eta)$, $q_2(\xi, \eta)$, and $q_3(\xi, \eta)$. For a particular set of fixed distribution of $\{\xi, \eta\}$, the

partition function is given by

$$Z(\xi, \eta) = \text{Tre}^{-\beta H(\xi, \eta)} = \int Du e^{-N \left[\frac{(q_3^2 - q_1^2 - q_2^2)}{2\beta J} - \frac{1}{N} \ln \text{Tre}^{-\beta H_{\text{eff}}} \right]}, \quad (4)$$

where $\beta = 1/T$ (T is the temperature), $Du \propto dq_1 dq_2 dq_3$, and

$$H_{\text{eff}} = \sum_{\nu}^{N_{\text{cl}}} \{ H_{J_1-J_2}^{\nu} - J [\xi_{\nu} (q_3 - q_1) + \eta_{\nu} (q_3 - q_2)] S_{\nu} \}. \quad (5)$$

In the thermodynamic limit ($N_{\text{cl}} \rightarrow \infty$), the steepest-descent method is used, which leads to $q_3 = q_1 + q_2$. The effective one-cluster problem becomes

$$H_{\text{eff}} = J_1 \sum_{(i,j)}^{n_s} \sigma_i \sigma_j + J_2 \sum_{\langle i,j \rangle}^{n_s} \sigma_i \sigma_j - J(\xi + \eta) q \sum_i^{n_s} \sigma_i, \quad (6)$$

where

$$q = q_1 = q_2 = \frac{1}{n_s} \left\langle \frac{\text{Tr} \left(\frac{\xi + \eta}{2} \sum_i^{n_s} \sigma_i e^{-\beta H_{\text{eff}}} \right)}{\text{Tre}^{-\beta H_{\text{eff}}}} \right\rangle_{\xi, \eta} \quad (7)$$

is the SG order parameter and $\langle \dots \rangle_{\xi, \eta}$ represents the average over the random variables ξ and η . Here, the intercluster disorder is treated within a mean-field approximation. However, it is important to remark that the short-range intracluster interaction is fully preserved, which leads to GF when $J_2/J_1 = 1$.

The free-energy per spin is obtained as

$$f = Jq^2 - \frac{1}{\beta n_s} \langle \ln \text{Tre}^{-\beta H_{\text{eff}}} \rangle_{\xi, \eta}. \quad (8)$$

The entropy per spin is given by

$$s = - \left(\frac{\partial f}{\partial T} \right) = \frac{\beta}{n_s} \left\langle \frac{\text{Tr} H_{\text{eff}} e^{-\beta H_{\text{eff}}}}{\text{Tre}^{-\beta H_{\text{eff}}}} \right\rangle_{\xi, \eta} - \frac{1}{n_s} \langle \ln \text{Tre}^{-\beta H_{\text{eff}}} \rangle_{\xi, \eta}, \quad (9)$$

and the intracluster spin-spin correlation is

$$\langle \sigma_i \sigma_j \rangle_{\xi, \eta} = \left\langle \frac{\text{Tr} \sum_{(i,j)}^{n_s} \sigma_i \sigma_j e^{-\beta H_{\text{eff}}}}{\text{Tre}^{-\beta H_{\text{eff}}}} \right\rangle_{\xi, \eta}. \quad (10)$$

III. RESULTS AND DISCUSSION

Numerical results are obtained by computing the single-cluster problem, given by Eqs. (6) and (7), in a self-consistent way. We consider clusters with n_s Ising spins on a checkerboard lattice with AF J_1 and J_2 interactions, as shown in Fig. 1(a). We define $r = J_2/J_1$, which is the GF parameter of the cluster. The SG phase is characterized by the SG order parameter $q \neq 0$ given by Eq. (7). In particular, a Landau expansion is used to locate the second-order phase transitions and the tricritical points, as discussed in the Appendix. The first-order phase transitions are obtained by comparing free energies of the PM and SG solutions. The magnetic behavior of the system with $J_2 = 0$ ($r = 0$ without GF) is studied in Sec. III A. In Sec. III B, we analyze the results with GF.

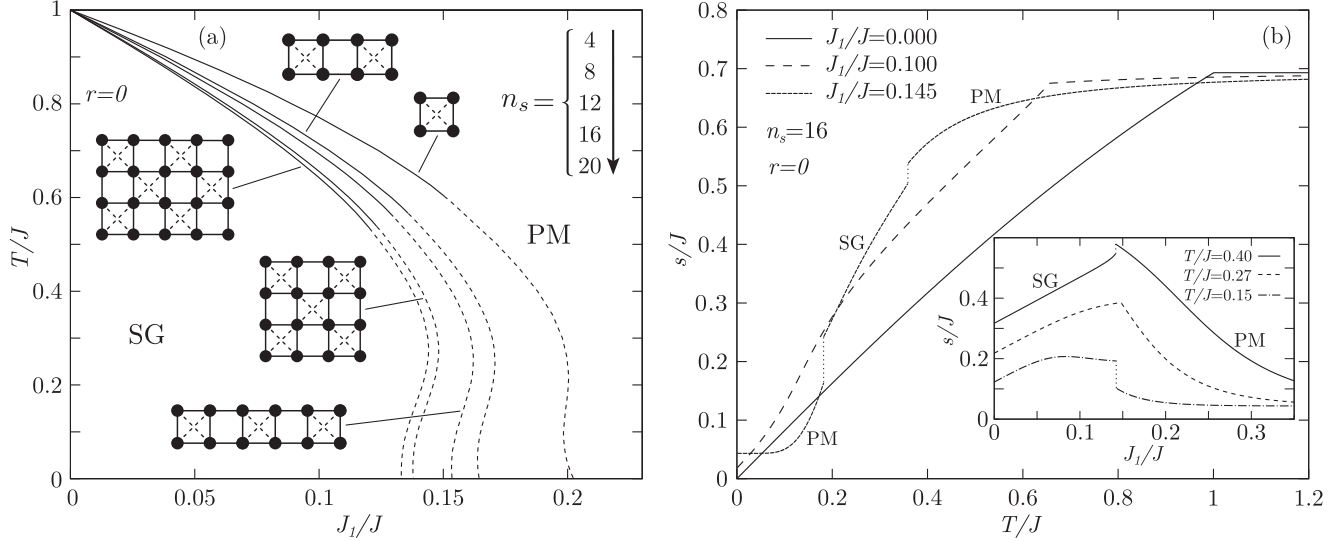


FIG. 1. Results for clusters without GF ($r = 0$). (a) Phase diagrams of T/J vs J_1/J for several cluster sizes, where the solid and dashed lines indicate second- and first-order transitions, respectively. Cluster shapes are also presented. (b) Entropy per spin as a function of temperature for $n_s = 16$. The inset exhibits the entropy as a function of J_1/J .

A. Clusters with first-neighbor AF interactions

In Fig. 1(a), a second-order phase transition separates the PM phase from the SG state when temperature diminishes for low intensities of J_1/J . The increase of J_1/J reduces the critical temperature T_f/J until a tricritical point, in which the transition becomes first-order. In the first-order region, a reentrant SG-PM transition appears, which is related to the IF phenomenon as discussed below. In particular, a second reentrance can occur at very low temperatures, introducing a SG ground state. These results indicate that the competition between AF intracluster interactions and intercluster disorder can drive to the IF. The J_1 interaction contributes to a fully compensated cluster moment, which is against the disordered interaction that is favored by a high cluster magnetic moment (uncompensated clusters). In this sense, the intercluster disorder leads to uncompensated clusters. Therefore, intercluster disorder and intracluster AF interactions cannot be completely satisfied simultaneously, which could be an additional source of frustration increasing the entropy of the SG phase.

For instance, the entropic behavior for $n_s = 16$ [see Fig. 1(b)] helps us to understand the effects of AF interactions in the SG phase. For $J_1/J = 0$, the entropy goes to zero when $T \rightarrow 0$, which is expected for a canonical SG system [22]. But in the presence of AF intracluster interactions, the entropy curve goes toward a finite value as $T \rightarrow 0$ inside the SG phase, as shown in Fig. 1(b) for $J_1/J = 0.1$. It is important to remark that this residual entropy is caused by the inability to satisfy the disordered and AF interactions at the same time. For large values of J_1/J , a PM ground state is found with a residual entropy of $S(T \rightarrow 0) = \ln(2)$ per cluster. However, for a certain range of J_1/J , the increase of temperature leads the PM system to a SG state. In other words, the cluster magnetic moments are thermally activated potentializing the disordered interactions, which can give rise to a SG state with higher entropy than the low-temperature PM phase, as shown in Fig. 1(b) for $J_1/J = 0.145$. In fact, the presence of AF intracluster interactions increases the SG

phase entropy, and, for a sufficiently low temperature, the PM phase has a lower entropy than the SG one [see the inset of Fig. 1(b)].

The intracluster spin-spin correlation $\langle \sigma_i \sigma_j \rangle_{\xi, \eta}$ between first neighbors can also be used to explain the effect of the AF interactions (see Fig. 2). In the absence of AF interactions, this spin-spin correlation within the SG phase is ferromagnetic, which is a consequence of the uncompensated states introduced by the intercluster disorder. However, the increase of J_1/J favors AF correlations. Therefore, the competition between disorder and J_1 interactions results in a conflicting situation that implies spin-spin correlation close to zero and a high entropy inside the SG phase. On the other hand, the increase in J_1/J can also lead to a PM phase with negative spin-spin correlation: $\langle \sigma_i \sigma_j \rangle_{\xi, \eta} \approx -1$. These results indicate

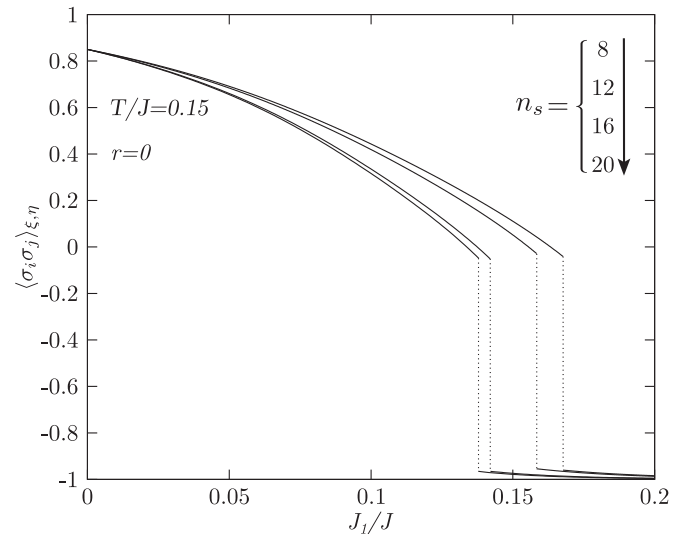


FIG. 2. Intracluster first-neighbor correlation as a function of J_1/J for several cluster sizes without GF. The cluster shapes are the same as in Fig. 1(a).

TABLE I. Relative degeneracy γ and ground-state entropy per spin for different n_s in the absence of disorder and $r = 1$. The cluster shapes are depicted in Fig. 1(a).

n_s	4	8	12	16	20
γ	1.667	2.657	3.433	4.092	4.675
$s(T=0)$	0.448	0.288	0.241	0.227	0.191

that the low-entropy PM phase is composed of compensated clusters.

We also investigate the cluster size outcome on the IF by considering various n_s , as displayed in Fig. 1(a). The SG region is reduced in the phase diagram as n_s increases. Furthermore, the cluster-size growth also leads to a reduction in the intracluster spin-spin correlation close to the phase transition, as exhibited in Fig. 2. This means that the increasing of the cluster size intensifies the effects of J_1 . We notice that the second reentrance, at very low temperatures, becomes less evident as n_s increases until it completely disappears for $n_s = 20$. In this way, the inverse reentrant transition becomes more pronounced for larger clusters. These findings are comparable to the results reported quite recently in a disordered cluster approach [19], in which the IF appears for a large enough cluster size and becomes more consistent as n_s increases. However, contrary to the present approach, the SK type of disordered interaction was considered in Ref. [19]. This suggests that our results are qualitatively insensitive to the choice of randomness.

We propose that the cluster-size effect could be analyzed by considering a relative degeneracy parameter $\gamma = \omega_{S_v \neq 0} / \omega_{S_v = 0}$, in which $\omega_{S_v \neq 0}$ (or $\omega_{S_v = 0}$) is the number of uncompensated (or compensated) cluster states. We find that γ is increased as n_s grows (see Table I). Interestingly, in disordered spin-1 systems with IF, a second reentrance was also found, but it disappears when the interacting states'

degeneracy is larger than that of the empty ones [6]. Although we analyze a different model, our results suggest that γ could be related to the relative degeneracy parameter proposed by Schupper and Shnerb [1,2] for the disordered spin-1 model. Thus, the cluster size could play an important role in inverse transitions.

B. Clusters with geometrical frustration

The presence of antiferromagnetic crossing (J_2) interactions introduces GF in the checkerboard lattice. In particular, for $r = 1$ the ground state is highly degenerated and constrained in such a way that each square with crossings has zero magnetization [26]. Additionally, the clusters used in our approach have a fully compensated ground state ($S_v = 0$) for $r = 1$ and $J = 0$.

The phase diagrams of Fig. 3(a) show that the IF does not appear for clusters with low n_s . The results of Fig. 3(b) indicate that the presence of intracluster GF leads to a low-temperature PM phase with higher entropy than the SG one, which prevents the IF transition for small clusters. To understand the effect of GF on the entropic content close to the low-temperature phase boundary, the inset of Fig. 3(b) exhibits entropy as a function of r for the PM and SG phases. The growth of r increases the entropy of both phases, which reaches a maximum close to $r = 1$. This indicates that the GF affects the SG phase entropy. In addition, this effect is more pronounced in the PM phase close to $r = 1$. In particular, we investigate how the system with geometrically frustrated clusters is affected by n_s .

Interestingly, the increase of n_s can bring again a reentrance [see Fig. 3(a) for $n_s \geq 16$], in which the SG entropy becomes higher than the low-temperature PM one [see Fig. 3(b)]. The cluster-size growth reduces the PM phase entropy (see Table I), and it also leads to an entropic inversion between the SG and PM phases close to the transition [see the insets of Fig. 3(b) for $n_s = 12$ and 20]. This means that the IF could appear in the geometrically frustrated case for large enough clusters. This

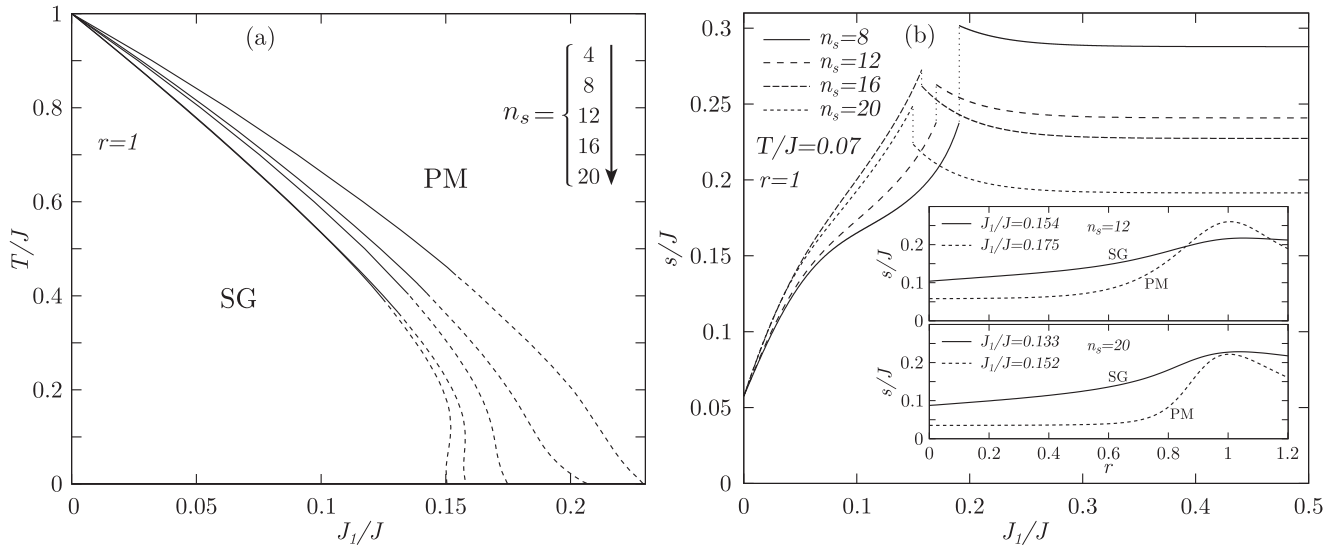


FIG. 3. Results for clusters with GF ($r = 1$). (a) Phase diagrams of T/J vs J_1/J , where solid and dashed lines represent first- and second-order transitions, respectively. (b) Entropy per spin as a function of J_1/J for $T/J = 0.07$. Insets show the entropy as a function of r at $T/J = 0.07$ for the SG and PM phases when $n_s = 12$ and 20. The cluster shapes are the same as Fig. 1(a).

result corroborates the arguments of Schupper and Shnerb, who proposed that a larger degeneracy of interacting states can be a key mechanism for inverse transitions [1,2]. However, contrary to previous works [1,2,6], here the relative degeneracy γ is a consequence of the cluster size, and it is not an additional (and rather artificial) parameter of the model.

IV. CONCLUSION

In summary, we have studied the interplay between GF and IF by adopting a cluster SG model in the checkerboard lattice. This approach enables us to tune the GF from the AF intracluster interactions J_1 and J_2 , while the disorder J comes from intercluster interactions. We find an IF transition in the absence of GF. The AF intracluster interactions compete with the intercluster disorder increasing the SG phase entropy. The increase of J_1 can also introduce a low-entropy PM phase with compensated clusters. At low temperatures, this PM phase has a lower entropy than the SG one.

When GF is considered, the IF occurs only for clusters higher than a critical size ($n_s \geq 16$). Regardless of the cluster compensation mechanism, GF increases the entropy of both phases: SG and PM. This increase is more pronounced on the disordered phase, which avoids a PM phase with lower entropy than the SG one at relatively small clusters. We propose that the cluster size growth leads to an increase in the relative degeneracy between compensated and uncompensated cluster states, in such a way that larger clusters can give an entropic advantage for the SG phase introducing IF. This hypothesis corroborates with the previous findings for spin-1 systems, in which the imposition of a relative degeneracy parameter favors the inverse transitions [1,2,6]. Here, the degeneracy

mechanism is a consequence of the AF disordered cluster framework. Although we study a specific model, our results enforce the idea that disordered systems with AF clusters (even with GF) are candidates to exhibit IF. In particular, we suggest that this cluster formalism could be a starting point for other studies of inverse transitions, including, for instance, random fields and quantum fluctuations.

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APPENDIX: LANDAU EXPANSION

The critical temperature can also be obtained from a Landau expansion for the free energy in powers of the order parameter q . Let us expand Eq. (8) through fourth order: $f = A_0 + A_2 q^2 + A_4 q^4 + O(q^6)$, where

$$A_2 = J \left(1 - \frac{\beta J}{n_s} \langle S^2 \rangle_{J_1-J_2} \right) \quad (\text{A1})$$

and

$$A_4 = -\frac{\beta^3 J^4}{2n_s} (\langle S^4 \rangle_{J_1-J_2} - 3\langle S^2 \rangle_{J_1-J_2}^2), \quad (\text{A2})$$

where $\langle \dots \rangle_{J_1-J_2}$ represents the thermal average for $H_{J_1-J_2} = J_1 \sum_{(i,j)} \sigma_i \sigma_j + J_2 \sum_{(i,j)} \sigma_i \sigma_j$. The second-order PM-SG phase transition occurs when $A_2 = 0$ with $A_4 > 0$, while the tricritical point is located when $A_2 = 0$ and $A_4 = 0$.

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