Ising ferromagnet in dimension five: Link and spin overlaps

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(Received 12 November 2012; published 1 February 2013)

In the simple [hyper]cubic five-dimension, near-neighbor-interaction Ising ferromagnet, extensive simulation measurements are made of the link overlap and the spin overlap distributions. These "two replica" measurements are standard in the spin glass context but are not usually recorded in ferromagnet simulations. The moments and moment ratios of these distributions (the variance, the kurtosis, and the skewness) show clear critical behaviors at the known ordering temperature of the ferromagnet. Analogous overlap effects can be expected quite generally in Ising ferromagnets in any dimension. The link overlap results in particular, with peaks at criticality in the kurtosis and the skewness, also have implications for spin glasses.

DOI: 10.1103/PhysRevE.87.022102 PACS number(s): 05.50.+q, 75.50.Lk, 64.60.Cn, 75.40.Cx

I. INTRODUCTION

As is well known, the upper critical dimension (ucd) for Ising ferromagnets is four. Here we show results of simulations for an Ising ferromagnet with near-neighbor interactions, on a simple [hyper]cubic lattice with periodic boundary conditions in dimension five, the next dimension up. The Hamiltonian is as usual,

$$\mathcal{H} = -J \sum_{ij} S_i S_j, \tag{1}$$

with spins i and j near neighbors. We will take $J = 1$ and will quote inverse temperatures $\beta = 1/T$.

All the principal properties of this system are well known. Recent consistent and precise estimates of the inverse ordering temperature β_c are 0.11391 [1], 0.113925(12) [2], 0.1139139(5) [3] from simulations, and 0.113920(1) [4] from high temperature series expansion (HTSE). We will use $\beta_c = 0.113915(1)$ as a compromise estimate. The susceptibility critical exponent and the effective correlation length exponent take the exact mean field values $\gamma = 1$ and $\nu = 1/2$, with a leading correction to scaling exponent $\theta = 1/2$ [5]. In the periodic boundary condition geometry, above the ucd the "effective length" is $L_{\text{eff}} = AL^{d/4}$, where A is a nonuniversal constant [1,6].

We analyze simulation data for the "two replica" observables link overlap and spin overlap, familiar in the Ising spin glass (ISG) context. It might seem curious to apply techniques developed for complex systems to the much simpler ferromagnet, particularly above the ucd, even though the observables can be defined in exactly the same way in a ferromagnet as in an ISG. Properties of the spin overlap at and beyond β_c have already been studied in the 3D Ising ferromagnet [7].

However, just because all the major parameters are well known it is convenient to use the 5D ferromagnet as a testbed for studying the critical behavior of various moments or moment ratios (the variance, the kurtosis, and the skewness) of both overlap distributions. The results should be generalizable *mutatis mutandis* to all Ising ferromagnets. The final aim is to establish the ground rules for the properties related to the link overlap near criticality in order to apply a similar methodology to complex systems, in particular to ISGs.

The link overlap [8], like the more familiar spin overlap, is an important parameter in ISG numerical simulations. In both cases, two replicas (copies) A and B of the same physical system, i.e., with identical sets of interactions between spins, are first generated and equilibrated; updating is then continued and the "overlaps" between the two replicas are recorded over long time intervals. The spin overlap at any instant t corresponds to the fraction $q(t)$ of spins S_i in A and B having the same orientation (S_i^A and S_i^B both up or both down), and the normalized overall distribution over time is written $P(q)$. The link overlap corresponds to the fraction $q_\ell(t)$ of links (or bonds or edges) ij between spins, which are either both satisfied or both dissatisfied in the two replicas; the normalized overall distribution over time is written $Q(q_\ell)$. The explicit definitions are

$$q(t) = \frac{1}{N} \sum_{i=1}^{N} S_i^A(t) S_i^B(t) \tag{2}$$

and

$$q_\ell(t) = \frac{1}{N_l} \sum_{ij} S_i^A(t) S_j^A(t) S_i^B(t) S_j^B(t), \tag{3}$$

where N is the number of spins in the system and N_l the number of links; spins i and j are linked, as denoted by ij. We will indicate means taken over time by $\langle \cdots \rangle$.

Equilibration and measurement runs were performed by standard heat bath updating on sites selected at random. The spin systems started with a random configuration, i.e., at infinite temperature, and were gradually cooled and equilibrated until they reached their designated temperatures, where they received a longer equilibration. For example, for $L = 10$ the systems at $\beta = 0.114$ saw roughly 10^6 sweeps before any measurements took place and the smaller systems at least 10^7 sweeps. Several sweeps were made between measurements and with a flip rate of about 27% near β_c, which means at least four sweeps between measurements. For $L = 10$ about 10^7 measurements were recorded at each temperature near β_c and considerably more for the smaller systems.

II. LINK OVERLAP

For any standard near-neighbor Ising ferromagnet with all interactions identical and with periodic boundary conditions,

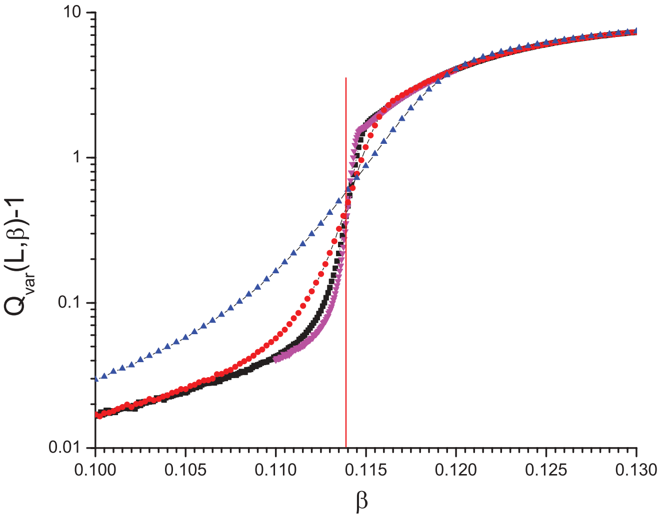

FIG. 1. (Color online) The Q variance [Eq. (6)] as a function of size and inverse temperature for the 5D near-neighbor ferromagnet. In this and all the following figures, the convention for indicating size is $L = 4$, blue triangles; $L = 6$, red circles; $L = 8$, black squares; $L = 10$, pink inverted triangles. In this and the following figures, errors are smaller than the size of the points unless stated otherwise. The red vertical line indicates the inverse ordering temperature $\beta_c = 0.113915$.

there is a simple rule for the mean link overlap in equilibrium $\langle q_\ell(\beta,L)\rangle$. If $p_s(\beta,L)$ is the probability averaged over time that any given bond is satisfied, then by definition the mean energy per bond is

$$|U(\beta,L)| \equiv 1 - 2p_s(\beta,L). \tag{4}$$

Because all bonds are equivalent

$$\langle q_\ell\rangle(\beta,L) = p_s^2 + (1-p_s)^2 - 2p_s(1-p_s) \equiv U(\beta,L)^2. \tag{5}$$

This rule is exact at all temperatures (we have checked this numerically), so it would appear at first glance that link overlap measurements present no interest in a simple ferromagnet as they contain no more information than the energy. However, the moments of the link overlap distribution reflect the structure of the temporary spin clusters, which build up in the paramagnetic state before β_c, and the domain structure in the ferromagnetic state beyond β_c. Thus, if at some instant t a cluster of parallel spins exists in replica A and a similar cluster in the same part of space exists in replica B, then the instantaneous $q_\ell(t)$ will be significantly higher than the time average $\langle q_\ell(t)\rangle$. The width of the overall distribution $Q(q_\ell)$ increases rapidly on the approach to β_c and we find phenomenologically that, as a consequence of the repeated occurrence of the cluster situation, around the critical temperature the distributions do not remain simple Gaussians but develop excess kurtosis and skewness, even though to the naked eye these deviations from pure Gaussian distributions are not obvious; for instance, no secondary peaks appear in the distributions.

We exhibit in Figs. 1–4 data at sizes $L = 4$, 6, 8, and 10 for the Q variance

$$Q_{\text{var}}(\beta,L) = \langle (q_\ell - \langle q_\ell\rangle)^2\rangle, \tag{6}$$

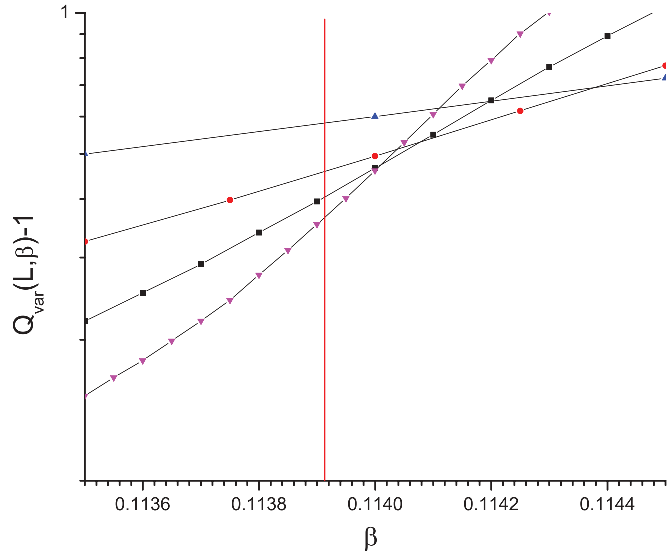

FIG. 2. (Color online) The Q variance as described in the legend of Fig. 1, in the region of the inverse ordering temperature β_c. Sizes coded as described in the legend of Fig. 1.

the Q kurtosis

$$Q_k(\beta,L) = \frac{\langle (q_\ell - \langle q_\ell\rangle)^4\rangle}{\langle (q_\ell - \langle q_\ell\rangle)^2\rangle^2}, \tag{7}$$

and the Q skewness

$$Q_s(\beta,L) = \frac{\langle (q_\ell - \langle q_\ell\rangle)^3\rangle}{\langle (q_\ell - \langle q_\ell\rangle)^2\rangle^{3/2}}. \tag{8}$$

The three Q moments and moment ratios follow the standard definitions for the moments of a distribution. For the Q variance we plot $\log[Q_{\text{var}}(\beta,L) - 1]$ so as to display the entire range of data. Figure 1 shows the behavior of the Q variance from high temperature through β_c to $\beta = 0.13$, well

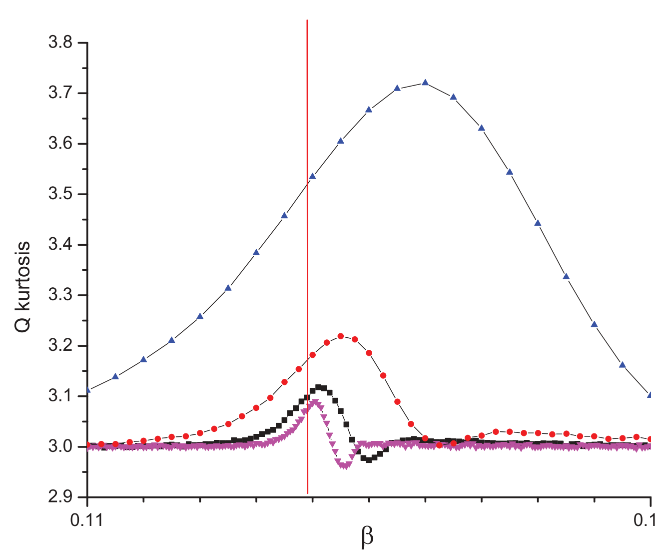

FIG. 3. (Color online) The Q kurtosis [Eq. (7)] for the 5D near-neighbor ferromagnet as a function of size and inverse temperature. Sizes coded as described in the legend of Fig. 1.

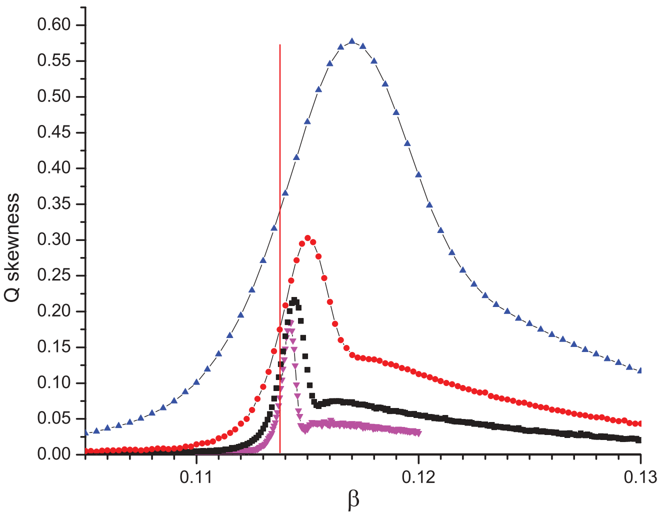

FIG. 4. (Color online) The Q skewness [Eq. (8)] for the 5D near neighbor ferromagnet as a function of size and inverse temperature. Sizes coded as described in the legend of Fig. 1.

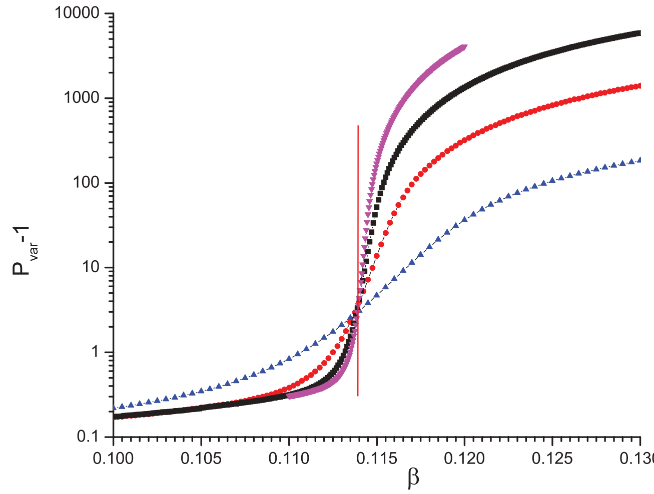

FIG. 5. (Color online) The P variance [Eq. (10)] for the 5D near-neighbor ferromagnet as a function of size and inverse temperature. Sizes coded as described in the legend of Fig. 1.

into the ordered state. Figure 2 shows the same data in the region near β_c.

It can be seen that the Q variance has clear critical behavior. Just as for standard "phenomenological couplings", such as the Binder cumulant or the correlation length ratio $\xi(\beta,L)/L^{5/4}$ (in the 5D case [1]), it is size independent at β_c to within a finite-size correction. As the Q variance is a phenomenological coupling in this particular system, it can be expected to have a similar form as a function of temperature in any ferromagnet, with the appropriate finite-size correction exponent. This makes the Q variance a supplementary phenomenological coupling for ferromagnets in general. As q_ℓ is a near-neighbor measurement like the energy, the distribution $Q(q_\ell)$ tends to equilibrate faster on annealing than a parameter such as the correlation length ξ.

The Q kurtosis has a more unusual form (Fig. 3). At temperatures well above or well below the critical temperature, it takes up the Gaussian value $Q_k(\beta) = 3$, but near criticality there is an excess Q kurtosis peak corresponding to a "fat tailed" form of the link overlap distribution. With increasing L, the width and strength of the peak decrease and the peak position $\beta_{\max}(Q_k)$ approaches β_c. In the present 5D ferromagnet case, the form of the temperature dependence evolves with L; with increasing L from a simple peak it tends to peak plus dip.

The Q skewness (Fig. 4) resembles the Q-kurtosis plot. The Q skewness starts at 0 (a symmetric distribution) at $\beta = 0$ and then develops a strong positive peak as a function of β in the region of β_c [so a distribution $Q(q_\ell)$ tilts toward high q_ℓ]. Again, the width and the strength of the peak decrease with increasing L. There is a weak indication of the beginning of a dip beyond the peak. The Q kurtosis and Q skewness can be expected to show qualitatively the same critical peak form in any ferromagnet.

For the moment, these observations are essentially phenomenological; it would be of interest to go beyond the argument given above in terms of correlated clusters of spins so as to obtain a full quantitative explanation for the details of the critical behavior of the $Q(q_\ell)$ distribution and its moments in finite L samples. Link overlap moment peaks in ISGs resemble these ferromagnet results [10], implying that the peak structure is a very general qualitative form of the behavior of link overlap distributions at an Ising magnet critical point.

The link overlap can be defined for vector spins [11] by

$$q_\ell = \frac{1}{N_l}\sum_{ij}\left[(\mathbf{S}_i^A\cdot\mathbf{S}_j^A)(\mathbf{S}_i^B\cdot\mathbf{S}_j^B)\right], \qquad (9)$$

which is invariant under global symmetry operations; the same link overlap critical properties as seen in Ising systems may well exist in XY and Heisenberg magnets also.

III. SPIN OVERLAP

As for the link overlap, one can also define various moments and moment ratios of the spin overlap distribution such as the P variance,

$$P_{\rm var}(\beta,L) = \langle q^2\rangle, \qquad (10)$$

and the P kurtosis,

$$P_k(\beta,L) = \langle q^4\rangle/\langle q^2\rangle^2, \qquad (11)$$

which is simply related to the Binder-like P cumulant $P_b(\beta,L) = [3 - P_k(\beta,L)]/2$.

The P variance in the ferromagnet has the phenomenological coupling form (Fig. 5); at β_c, the P variance tends to an L-independent value with a finite-size correction. As the temperature goes to zero the P variance will tend to L^d. The P kurtosis has a different phenomenological coupling form (Fig. 6), a peak before a sharp drop to 1, corresponding to the $P(q)$ distribution becoming "fat tailed" before and at β_c before taking on a two-peak structure in the ordered state [7]. This is in contrast to the magnetization M kurtosis (usually expressed as the Binder cumulant) in ferromagnets or the standard P kurtosis in ISGs, which both drop regularly from the Gaussian value 3 toward the two peak value 1 with increasing order.

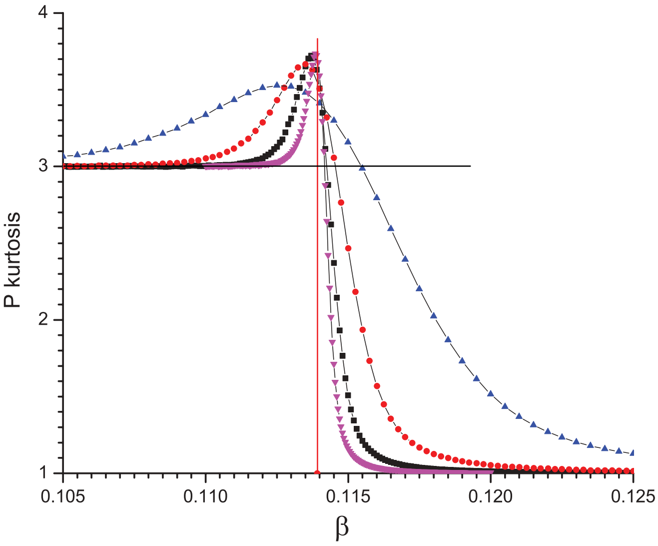

FIG. 6. (Color online) The P kurtosis [Eq. (11)] for the 5D near-neighbor ferromagnet as a function of size and inverse temperature. Sizes coded as described in the legend of Fig. 1.

However, it can be noted that the temperature variation of the kurtosis for the chiral order parameter in Heisenberg spin glasses has the same general form as the present ferromagnetic P kurtosis, the distribution becoming fat tailed above the ordering temperature [9].

As the distributions $P(q)$ in equilibrium are by definition symmetrical about $q = 0$, the P skewness is always zero. However, for the one-sided distribution of the absolute value of $|q|$, other parameters can be defined, in particular, the absolute P kurtosis,

$$P_{|q|,k}(\beta,L) = \frac{\langle(|q| - \langle|q|\rangle)^4\rangle}{\langle(|q| - \langle|q|\rangle)^2\rangle^2}, \tag{12}$$

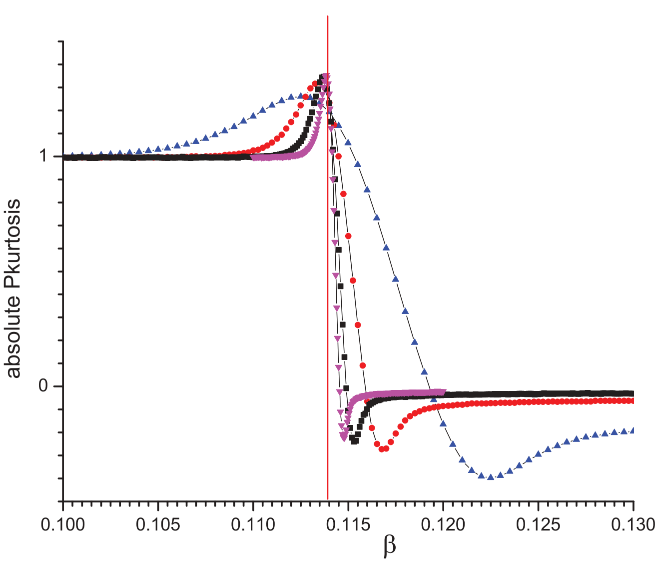

FIG. 7. (Color online) The absolute P kurtosis, $P_{|q|,k}$ [Eq. (12)], for the 5D near-neighbor ferromagnet as a function of size and inverse temperature. Sizes coded as described in the legend of Fig. 1.

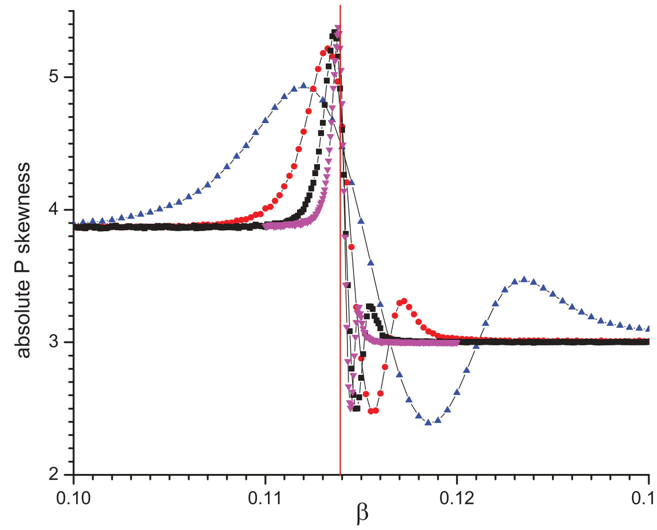

FIG. 8. (Color online) The absolute P skewness, $P_{|q|,s}$ [Eq. (13)], for the 5D near-neighbor ferromagnet as a function of size and inverse temperature. Sizes coded as described in the legend of Fig. 1.

and the absolute P skewness,

$$P_{|q|,s}(\beta,L) = \frac{\langle(|q| - \langle|q|\rangle)^3\rangle}{\langle(|q| - \langle|q|\rangle)^2\rangle^{3/2}}. \tag{13}$$

The absolute P kurtosis and the absolute P skewness in the ferromagnet have rather complex phenomenological coupling temperature-dependence patterns, with very weak finite size corrections at β_c (Figs. 7 and 8). If the weak finite-size correction is a general property for these parameters, it could be usefully exploited so as to obtain high-precision estimates of ordering temperatures in systems where these temperatures are not well known.

The spin overlap properties do not transport from the ferromagnet into ISG systems in the same manner as the link overlap properties do because the P variance takes on a different status: in an ISG, q^2 becomes the order parameter.

IV. CONCLUSION

The standard near-neighbor interaction Ising ferromagnet on a simple [hyper]cubic lattice in dimension five has been used as a test case in order to demonstrate the critical form of the temperature variations of observables related to the link overlap and the spin overlap, parameters developed in the ISG context and not generally recorded in ferromagnet simulations. The moments of the link and spin overlap distributions, $Q(q_\ell)$ and $P(q)$, show a rich variety of temperature variations, with specific critical behaviors. The temperature dependence of the link overlap kurtosis and the link overlap skewness show peaks at criticality that are "evanescent" in the sense that they will disappear in the large-size thermodynamic limit. The present results validate the assumption that these observables show true critical temperature dependencies. A temporary cluster phenomenon is proposed as determining the evolution of the link overlap distributions. If correct, this mechanism is quite general, so we expect the critical peaks in the Q kurtosis and the Q skewness to be present in the entire class of Ising ferromagnets, not only those in dimensions above the ucd, and plausibly in vector spin ferromagnets also. Beyond the class of ferromagnets, it can be noted that link overlap Q kurtosis and Q skewness critical peaks have also been observed [10] in Ising spin glasses.

ACKNOWLEDGMENTS

The computations were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at High Performance Computing Center North (HPC2N).

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