Phase Diagram of the three-dimensional Gaussian Random Field Ising Model: A Monte Carlo Renormalization Group Study

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With the help of the replica exchange Monte Carlo method and the improved Monte Carlo renormalization-group scheme, we investigate over a wide area in the phase diagram of the Gaussian random field Ising model on the simple cubic lattice. We found that the phase transition at a weak random field belongs to the same universality class as the zero-temperature phase transition. We also present a possible scenario for the replica symmetry-breaking transition.

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The random field Ising model in three dimension[1] has been intensively studied for over 30 years by experimental, theoretical, and numerical methods. But there are still some unanswered questions. One of the questions is as follows: Does the phase transition for different strengths of random field belong to the same universality class? Critical behavior at the strong field region[2,3] and zero-temperature line[4] has been studied numerically by several authors, and from the fact that the observed value of the critical exponent \( \theta \) is positive,[4] the existence of the zero-temperature random fixed point (ZRFP) seems unquestionable. Together with the fact that random field is relevant at the pure critical point,[1] the renormalization-group (RG) flow in the temperature-field phase diagram can be depicted as in Fig. 1. The behavior of the RG flow in the intermediate region is unknown and it is unclear whether the ZRFP governs the whole phase transition or not.

Another question is as follows: Is there a glasslike phase near the critical line in the phase diagram? Theoretical studies based on the replica formalism[1] have predicted the presence of a glasslike phase which is characterized by replica symmetry breaking near the transition temperature.[1] But owing to the unphysical \( n \to 0 \) limit in the theory, interpretation of the result is not trivial.

For the investigation of these problems, direct observation of the RG flow may be the most powerful method. In the present work, we numerically observed the RG flow of the Gaussian random field Ising model over a wide region in the phase diagram using an improved Monte Carlo renormalization-group (MCRG) scheme,[5] which is a very simple and sophisticated method. We used the following model in the Monte Carlo simulations:

\[
H = \sum_{<ij>} S_i S_j + h \sum_i S_i h_i,
\]

where the first summation runs over all the nearest-neighbor pairs of the sites on an \( L \times L \times L \) simple cubic lattice (up to \( L = 16 \)) with a periodic boundary condition, and \( h_i \) is a random Gaussian variable whose average is 0 and variance is 1. We measured the following quantities:

\[
T_L = \frac{[(M^2 - \langle M^2 \rangle)^2]}{2\langle M^2 \rangle^2},
\]

\[
S_L = \frac{[\langle M^2 \rangle - \langle \langle M^2 \rangle \rangle^2]}{2\langle M^2 \rangle^2},
\]

where \( M \) denotes magnetization, the symbol \( \langle \cdot \cdot \cdot \rangle \) and \( [\cdot \cdot \cdot] \) denote thermal and en-
semble averages, respectively. $T_L$ and $S_L$ are the amplitudes of thermal and sample-to-sample fluctuations, respectively, of the rescaled block spin $M/\sqrt{\langle M^2 \rangle}$ defined on an $L \times L \times L$ block. Thus $T_L$ and $S_L$ reflects the renormalized temperature and strength of the random field, respectively. If the ZRFP governs the whole critical line, the flow of $T_L$ and $S_L$ will become the one depicted in Fig. 2(a). On the other hand, if there exists another fixed point, the flow will become the one depicted in Fig. 2(b). Note that, in the paramagnetic phase, thermal and sample-to-sample fluctuations are on the same order $O(L^{3/2})$ and there are a set of “high temperature fixed points” on a line $T_L + S_L = 1$, where both fluctuations are Gaussian. The position of the fixed point depends on the ratio between the two amplitudes.

In the Monte Carlo simulation, we used a single-spin-flip Metropolis update and the replica exchange method. In a replica exchange procedure, an exchange for all adjacent temperature pairs was tried. The exchange procedure was performed for every two Metropolis sweeps. We used 20 replicas for all field realizations. Temperatures for all replicas were chosen so that the replica exchange occurs with modest frequency and the highest temperature is well above the transition temperature where the single-spin-flip provides good ergodicity. Figure 3 shows the region in the phase diagram where the simulations were carried out in the present work, together with other recent numerical studies. The case $h = 1.3$ was the hardest to relax, in which we used 88 000 Monte Carlo steps (discarding the initial 8000 steps) for each field realization. We checked that two kinds of initial states, all spins up and down, give the same thermal averages of $M$ within statistical errors, thus the system is well equilibrated. This result is remarkably fast compared to the simulation in which only the Metropolis update was used and $2 \times 10^6$ steps were needed to fulfill the same criterion. We used 120 different random field realizations for each $L$ and $h$. This number of samples is rather small compared to other recent numerical works. But our aim in the present work is to draw qualitative conclusions, not quantitative estimates of critical exponents, and it was enough for this purpose.

Figure 4 shows the flow of $T_L$ and $S_L$ on a logarithmic scale. All lines are drawn from $(T_L, S_L)$ to $(T_2L, S_2L)$ with $L = 4$ (thin lines) and $L = 8$ (bold lines). The RG flow of both sizes are consistent, which indicates that the finite-size effect is small enough and the final destination of the RG flow can be safely predicted. Thus one can see that there are no fixed points in the intermediate region, and the renormalization flow which starts at the weak-field region is eventually attracted to the low-temperature region $T_L < 0.01$. Figure 5 shows the RG flow near the ZRFP. The precise position of the ZRFP $(0, S_\ast)$ is hard to estimate, owing to its proximity to the low-temperature fixed point $(0, 0)$. We only performed a rough estimate of the critical value $S_\ast$ as $0 \leq S_\ast < 0.01$, which is consistent with the result of the zero-temperature simulation. $S_\ast = 0.003(2)$. Thus Figs. 4 and 5 indicate that the ZRFP governs the whole phase-transition line.

Now let us consider the possibility of a first-order transition. If the transition is of first order, an ensemble distribution of $\langle M^2 \rangle$ will exhibit a double-peak structure and a plot of $S_L$ will develop a sharp peak at the transition temperature. But no such behavior was observed in the present work. Note that when we observe a single sample at zero temperature and varying $h$, the system jumps between different ground states and there are many discontinuous transition points on the $h$ axis. Similar behavior will be observed in the low-temperature region and some sample may exhibit the double-peak behavior. However, if ensemble distri-
distribution of the ground-state magnetization at zero temperature does not exhibit double-peak behavior, an ensemble average of the ground state magnetization will not change discontinuously and the transition is of second order, as is the result of Ref. [9].

Figure [3] shows plots of $S_L$ against temperature at $h = 1.3$. The bold line denotes the expected behavior in the $L \to \infty$ limit, assuming that the basin of the fixed point $S_L = 1, T_L = 0$ has a finite measure in Fig. [3](a). $S_\infty$ reaches its maximum value 1 slightly above the critical temperature and remains 1, then discontinuously drops to a critical value $S_*$ at the critical temperature. Note that $S_L$ is a similar quantity to the replica interaction term $\phi \phi^*_2$ in the $\phi^4$ model based on the replica formalism, in which divergence of the coefficient of $\phi \phi^*_2$ at the paramagnetic phase is reported [8]. In the $S_\infty = 1$ region, thermal fluctuation of the magnetization becomes more and more negligible compared to its absolute value as $L$ becomes large. This means that the breadth of each valley in the free-energy landscape becomes negligible compared to the distances between each valley. In this limit, an infinitesimal change of $h$ or $T$ will drive the system out of a valley and into another valley. This could be a possible scenario for the replica symmetry-breaking transition [9] and can be tested numerically by checking the following inequality:

$$\lim_{\Delta \to 0} \lim_{L \to \infty} \left[ \langle M(h) \rangle \langle M(h + \Delta) \rangle \right] \neq \left[ \langle M(h) \rangle \right]^2,$$

(4)

with a very careful finite-size scaling analysis.

In conclusion, we performed a replica exchange Monte Carlo simulation of the Gaussian random field Ising model in three dimensions and, using an improved MCRG scheme, we found that the phase transition at the weak random field belongs to the same universality as the zero-temperature phase transition, and we presented a possible scenario for the replica symmetry-breaking transition.

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1 For reviews, see T. Nattermann and P. Rujan, Int. J. Mod. Phys. B3,1597 (1989); T. Nattermann, in Spin Glasses and Random Fields edited by A. P. Young (World Scientific, Singapore, 1997).
2 H. Rieger, Phys. Rev. B 52, 6659 (1995).
3 J. Matcha, M. Newman and L. Chayes, Phys. Rev. E 62, 8782 (2000).
4 M. R. Swift, A. J. Bray, A. Maritan, M. Cieplak, and J. R. Banavar, Europhys. Lett. 38, 273 (1997).
5 M. Itakura, Phys. Rev. E 61, 5924 (2000).
6 K. Hukushima and K. Nemoto, J. Phys. Soc. Jpn. 65, 1604 (1996).
7 We also observed several other quantities such as $\langle S(k_1)S(-k_1) \rangle / \langle M^2 \rangle$ and $\langle S(k_1)S(-k_1) \rangle / \langle M^2 \rangle$ where $S(k) = \sum r S_r \exp(ikr)$ and $k = (2\pi/L,0,0)$, but critical values of these quantities are also very close to the one at the low-temperature fixed point.
8 When $\alpha \neq \beta$, $\langle \phi^2 \phi^*_2 \rangle = \langle \phi^2 \rangle^2$ for finite systems, while $S_L = \langle \phi^2 \rangle^2 / 2 - 1$ if we define $\phi \equiv M / \sqrt{\langle M^2 \rangle}$.
9 E. Brézin and C. De Dominicis, Eur. Phys. J. B 19, 467 (2001).
10 M.J. Alava, P.M. Duxbury, C.F. Moukarzel and H. Rieger in Phase transition and Critical Phenomena, vol. 18, edited by C. Domb and J.L. Lebowitz (Academic, London, 2001).
FIG. 1. Schematic renormalization flow in the temperature-field phase diagram.

FIG. 2. Expected renormalization flow of $T_L$ and $S_L$ for the case of (a) the zero-temperature random fixed point only and (b) another fixed point in the intermediate region. L, P, and $R_x$ denote low-temperature, pure-critical, and random fixed points, respectively.

FIG. 3. Regions in the $T$-$h$ phase diagram where simulations were carried out in the present work, together with other recent numerical works.

FIG. 4. Observed renormalization flow of $T_L$ and $S_L$. The bold dashed line is an approximate phase boundary. Note the logarithmic scale of the plot. Errors are smaller than the size of symbols, unless errorbars are explicitly shown.

FIG. 5. Renormalization flow of $T_L$ and $S_L$ near the ZRFP. The bold dashed line is an estimated position of ZRFT in Ref.[4].
FIG. 6. Plots of $S_L$ against temperature $T$ for $h = 1.3$. The bold line is the expected behavior for the $L = \infty$ case.