Random Fixed Point of Three-Dimensional Random-Bond Ising Models

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The fixed-point structure of three-dimensional bond-disordered Ising models is investigated using the numerical domain-wall renormalization-group method. It is found that, in the $\pm J$ Ising model, there exists a non-trivial fixed point along the phase boundary between the paramagnetic and ferromagnetic phases. The fixed-point Hamiltonian of the $\pm J$ model numerically coincides with that of the unfrustrated random Ising models, strongly suggesting that both belong to the same universality class. Another fixed point corresponding to the multicritical point is also found in the $\pm J$ model. Critical properties associated with the fixed point are qualitatively consistent with theoretical predictions.

KEYWORDS: domain wall renormalization group, fixed point, random system, spin glass, MC simulation

The influence of quenched disorder on model systems has attracted considerable interest in the field of statistical physics. The first remarkable criterion was given by Harris, who claimed that if the specific-heat exponent $\alpha_{\text{pure}}$ of the pure system is positive, disorder becomes relevant, implying that a new random fixed point governs critical phenomena of the random system. One of the simplest models belonging to such a class is the three-dimensional ($3D$) Ising model. Critical exponents associated with the random fixed point have been investigated for dilution-type disorder by experimental and theoretical approaches. Recently, extensive Monte Carlo (MC) studies have clarified that the critical exponents of the $3D$ site-diluted Ising model are independent of the concentration of the site dilution $p$, suggesting the existence of a random fixed point. These results were obtained by carefully taking into account correction for finite-size scaling, unless the exponents clearly depend on $p$. Experimentally, the critical exponents of randomly diluted antiferromagnetic Ising compounds, Fe$_x$Zn$_{1-x}$F$_2$ and Mn$_x$Zn$_{1-x}$F$_2$, are distinct from those of the pure $3D$ Ising model.

While the existence of the random fixed point has been established for the $3D$ site-diluted Ising model, the idea of the universality class for random systems, namely classification by fixed points, has not been explored yet as compared with various pure systems. In particular, the question as to whether the random fixed point is universal irrespective of the type of disorder or not is a non-trivial problem. In the present work, we study critical phenomena associated with the ferromagnetic phase transition in $3D$ site- and bond-diluted and $\pm J$ Ising models. The main purpose is to determine the fixed-point structure of $3D$ random-bond Ising models by making use of a numerical renormalization-group (RG) analysis. Our strategy is based on the domain-wall RG (DWRG) method proposed by McMillan. This method has been applied to a $2D$ frustrated random-bond Ising model, where there is no random fixed point, and recently to a $2D \pm J$ frustrated random-bond three-state Potts model, which displays a non-trivial random fixed point. In this paper, we show systematic RG flow diagrams for $3D$ random Ising spin systems, which convinces us of the existence of the random fixed point.

Let us first explain briefly the RG scheme and the numerical method used by us. In the DWRG scheme, the following domain-wall free energy $\Delta F_J$ of a spin system on a cube with the size $L$ is regarded as an effective coupling associated with a length scale $L$ for a particular bond configuration, denoted by $J$:

$$\frac{\Delta F_J(T)}{T} = \ln \frac{Z_p(T)}{Z_{\text{AP}}(T)}$$

where $Z_{\text{AP}}(T)$ is the partition function of the cube at temperature $T$ under (anti-) periodic boundary conditions for a given direction, while the periodic boundary conditions are imposed for the remaining directions. In disordered systems, the distribution $P(\Delta F)$ of the effective couplings over the bond configurations is considered to be a relevant quantity. Therefore, in the DWRG scheme, we are interested in how the distribution is renormalized as $L$ increases. In the ferromagnetic phase, the expectation value of the distribution approaches infinity as $L$ increases, while it vanishes in the paramagnetic phase. Fixed points are characterized by an invariant distribution of the coupling under a DWRG transformation, namely, increasing $L$. For example, the unstable fixed-point distribution corresponding to the pure-ferromagnetic phase transition is a delta function with a non-zero mean. The random fixed point, if any, is expected to have a non-trivial distribution with a finite width.

It is convenient to consider typical quantities characterizing the distribution $P(\Delta F)$, instead of the distribution itself. We discuss here the mean $\Delta F$ and the width $\sigma(\Delta F)$ of the distribution which are evaluated as

$$\Delta F = \int d\Delta F \; \Delta F \; P(\Delta F),$$

$$\sigma(\Delta F) = \sqrt{\int d\Delta F (\Delta F - \langle \Delta F \rangle)^2 P(\Delta F)}.$$
\[ \sigma^2(\Delta F) = \frac{\Delta F^2}{\Delta F^2}, \] (3) respectively. Using these quantities, we define two reduced parameters, \( r = \sigma(\Delta F)/\Delta F \) and \( t = T/\Delta F \), as in the previous works. The renormalized parameters \((r(L), t(L))\) of the length scale \( L \) are estimated numerically with bare parameters in a model Hamiltonian fixed. Then, the RG flow is represented by an arrow connected from the point \((r(L), t(L))\) of size \( L \) to \((r(L'), t(L'))\) of a larger size \( L' \). Fixed points should be observed as points where the position is invariant under the RG transformation. Linearizing the flow about a fixed point \((r^*, t^*)\), we obtain

\[ \begin{pmatrix} r(L') - r^* \\ t(L') - t^* \end{pmatrix} = \mathbf{T} \begin{pmatrix} r(L) - r^* \\ t(L) - t^* \end{pmatrix}, \] (4)

where \( \mathbf{T} \) is a RG transformation matrix whose eigenvectors are scaling axes of the RG flow. The matrix elements of \( \mathbf{T} \) as well as the fixed point \((r^*, t^*)\) can be determined by least-squares fitting from the data point numerically obtained. The critical exponents \( y \) are obtained as \( \log \lambda/\log(L'/L) \) with the eigenvalue \( \lambda \) of \( \mathbf{T} \).

We consider Ising models with quenched disorder which is defined on a simple cubic lattice. The model Hamiltonian is

\[ \mathcal{H}(J_{ij}, S_i) = -\sum_{(ij)} J_{ij} S_i S_j, \] (5)

where the sum runs over nearest-neighbor sites. In order to obtain the domain-wall free energy, we use a recently proposed MC method which enables us to evaluate the free-energy difference directly with sufficient accuracy. In the novel MC algorithm, we introduce a dynamical variable specifying the boundary conditions, which is the sign of the interactions between the first and the last layer of the cube for the given direction. The algorithm is based on the exchange MC method, sometimes called the parallel tempering, which turns out to be reasonably efficient for randomly frustrated spin systems.

![Flow diagram for the 3D unfrustrated bond-diluted Ising model.](image)

Fig. 1. Flow diagram for the 3D unfrustrated bond-diluted Ising model. The random fixed point is found numerically at \((0.63(2), 1.77(5))\). The bold arrows indicate the eigenvectors, whose exponents are \( y_1 = 1.47(4) \) and \( y_2 = -1.3(4) \).

First we study a 3D bond-diluted Ising model, which is given by eq. \ref{eq:3Dbond} with the bond distribution, \( P(J_{ij}) = p\delta(J_{ij} - J) + (1 - p)\delta(J_{ij}) \). The bond concentrations studied are \( p = 1.00, 0.90, 0.65, 0.45 \) and 0.35 with the system sizes \( L = 8 \) and \( L = 12 \). Sample averages are taken over 128–1984 samples depending on the size and the concentration. Errors are estimated from statistical fluctuation over samples.

![Phase diagram of the 3D random-bond Ising models with the bond (triangle) and the site (box) dilution.](image)

Fig. 2. Phase diagram of the 3D random-bond Ising models with the bond (triangle) and the site (box) dilution. In the inset, a schematic flow diagram for the diluted Ising models is shown as a function of temperature and disorder. The fixed points and the RG flow are indicated.

The transition temperatures are estimated by a naive finite-size scaling assumption with the correlation-length exponent \( \nu \), namely, the crossing point of \( \Delta F \) with \( L = 8 \) and 12 as a function of temperature is located on \( T_c \). This scaling form is similar to that of the Binder parameter frequently used. The estimated \( T_c \) is shown in Fig. 2. The exponent \( \nu \) obtained by the scaling depends significantly on the concentration...
p, similar to those observed as an effective exponent in the MC simulation of the site-disordered Ising model. It is found from the RG flow diagram that the system has a subleading scaling parameter which gives rise to a systematic correction to the scaling. Therefore, we conclude that the continuously varying exponent observed in the naive scaling is due to the subleading parameter.

We also investigate a 3D site-diluted Ising model by the same procedure as in the bond-diluted Ising model described above. The model is given by eq. (5) but with the bond $J_{ij} = J_0 \epsilon_i \epsilon_j$ and the distribution, $P(\epsilon_i) = p\delta(\epsilon_i - 1) + (1-p)\delta(\epsilon_i)$. As shown in Fig. 3, there exists a random fixed point, which is consistent with the universality scenario observed in this 3D site-diluted Ising model. In the MC simulation, the correction to the scaling becomes smaller around $p = 0.80$. This can be explained by the finding that the random fixed point we found is located on the position near the bare coupling with $p = 0.80$. An interesting point to note is that the position of the fixed point is close to that observed in the 3D bond-diluted Ising model, though the corresponding bare parameters such as the concentration $p$ and the temperature differ between these two models, as seen in Fig. 2. This finding implies that the random fixed point is universal for a large class of the 3D unfrustrated random Ising models.

Next we consider a $3D \pm J$ Ising model, where the interactions $J_{ij}$ are randomly distributed according to the bimodal distribution, $P(J_{ij}) = p\delta(J_{ij} - J) + (1-p)\delta(J_{ij} + J)$. The multi-spin coding technique can be easily implemented in this model. For that purpose, we consider 32 temperature points in the exchange MC simulation. In this model, the ferromagnetically ordered state survives at low temperatures up to a critical concentration, recently estimated at $p_c = 0.7673(3)$, while below $p_c$ a spin glass (SG) phase appears. We estimate the domain-wall free energy with $L = 8$ and 12 for a wide range of concentration $p$ including the critical concentration. Sample averages are taken over 240 – 6800 samples depending on the size and the concentration.

We show in Fig. 4 the RG flow diagram for the $3D \pm J$ Ising SG model. The arrow connects results for $L = 8$ and $L' = 12$. Here, we again find the random fixed point $R$ as an attractor along the ferromagnetic phase boundary. The position of $R$ is also close to that observed in the diluted Ising models. This finding indicates that both belong to the same universality class as the ferromagnetic phase transition. In other words, the renormalized coupling constants (or coarse-grained spin configurations) are independent of the details of the microscopic Hamiltonian and of whether it is frustrated or not. One of the inherent characteristics of the $\pm J$ model is the existence of a highly symmetric line, which we call the Nishimori line. There were several theoretical works concerning the Nishimori line. It was suggested by the $\epsilon$-expansion method and a symmetry argument that the multicritical point must be located on the line. This was confirmed by MC simulations and high-temperature series expansions. As shown in Fig. 4, we also observe a fixed point, denoted by $N$, corresponding to the multicritical point, where both scaling axes have a positive eigenvalue. One of the scaling axes governed by the larger eigenvalue at $N$ almost coincides with the Nishimori line, which is in agreement with the predictions by the $\epsilon$-expansion.

As seen in Fig. 5, the estimated critical temperatures for the concentrations simulated are consistent with those obtained by the large-scale MC simulations up to size $L = 101$. Our analysis can also be performed for the SG transition at smaller values of $p$. The SG transition temperature $T_{SG}$ is determined from the crossing of $\sigma(\Delta F)$. The value of $T_{SG}$ at $p = 0.50$ is in good agreement with the recent estimation. Along the ferromagnetic phase boundary, it is natural to expect that there exists another fixed point $Z$ at zero temperature, which separates the ferromagnetic phase from the SG one. Because the eigenvalues of the RG matrix at $N$ are positive for both scaling axes, the thermal axis would be irrelevant in contrast to the diluted Ising models, namely,
an irrelevant flow into the zero-temperature fixed point \( Z \) originates at \( N \), as shown in the inset of Fig. 5. The zero-temperature fixed point governs the critical behavior between the ferromagnetic and SG phase. In the present study, however, we cannot reach temperatures that are sufficiently low to extract the zero-temperature fixed point. A modern optimization technique such as a genetic algorithm would be useful in searching for the location of the fixed point.

![Phase diagram of the 3D ± J Ising SG model.](image)

Fig. 5. Phase diagram of the 3D ± J Ising SG model. Open triangles are transition temperature estimated in the present work. The SG transition temperatures marked by the solid triangles at \( p = 0.50 \) and 0.76 are determined from \( \sigma(\Delta F) \). The open circles represent estimations by the nonequilibrium MC relaxation method. The dotted line represents the so-called Nishimori line. A schematic flow diagram for the ± J model is drawn in the inset. The fixed points \( R \) and \( N \), and the RG flow around them are supported in the present work.

Now we comment on the correction to the finite-size scaling. In order to obtain the critical exponent, one uses a range of the system size frequently independent of the bare parameters in the model Hamiltonian. When the system has a subleading scaling parameter, it causes systematic corrections to the scaling. However, it is not known how such corrections affect the leading scaling \textit{a priori}. The RG flow diagram gives a good indication of necessity and justification for corrections to the leading scaling term. Once the fixed-point structure of interest is clarified from the flow, one of the best numerical approaches to obtain the critical exponents, within restricted computer facilities, is to choose a model parameter close to the fixed Hamiltonian.

In experiments, the 3D ± J Ising model is approximately realized in a mixed compound with strong anisotropy such as Fe\(_2\)Mn\(_{1-x}\)TiO\(_3\). Our findings suggest that the critical phenomena of the compound Fe\(_2\)Mn\(_{1-x}\)TiO\(_3\) near \( x \approx 1 \) belong to the same universality class as the 3D random Ising models. We expect that various random Ising systems such as a mixed Ising spin compound Fe\(_2\)Co\(_{1-y}\)Fe\(_2\) though beyond the scope of the present study, are also categorized into the same universality class.

In conclusion, we have studied the fixed-point structure of the 3D random-bond Ising models using the numerical DWRG method. We have found in the ± J Ising model, a random fixed point besides the pure and multicritical ones along the ferromagnetic phase boundary. Furthermore, the observed random fixed point is found to be very close to that of the 3D non-frustrated dilute Ising models, while bare parameters in the model Hamiltonians differ entirely. This fact strongly suggests that there exists a universal fixed point characterizing the 3D disordered ferromagnetic Ising model irrespective of the type of disorder. The present work is, to our knowledge, the first of its kind performed for determining the fixed-point structure of a 3D random spin system. We consider that the present numerical RG approach is quite useful for understanding the universality class of random spin systems, including spin glasses.

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