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Crossover effects in dilute magnetic materials by finite-time dynamics method☆

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HIGHLIGHTS

- We derive the scaling function to probe critical behavior.
- We use finite-time dynamics method in three-dimensional bond-diluted Ising model.
- Results support a single universality class and smaller dynamic critical exponent.

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ABSTRACT

Crossover phenomena are ubiquitous in disordered system. However, the crossover effects from the competition between different fixed points make it hard to identify the asymptotic scaling regime controlled by the random fixed point. Therefore, the analyses on the crossover effects are of great importance to understand phase transition in dilute magnetic materials. In this paper, we derive the scaling function characterizing the crossovers to probe critical behavior. According to these, we show an alternative method to locate the asymptotic critical region in the quenched random systems in the finite-time dynamics frame. For the three-dimensional bond-diluted Ising model, the asymptotic critical exponents are identified with $\nu = 0.686(1)$, $\beta = 0.356(6)$, $\alpha = -0.057(3)$, $\gamma = 1.345(20)$, $z = 2.170(11)$ at middle bond concentration $p = 0.7$ from the effective ones describing the approach to the asymptotic regime for weak dilution ($p = 0.9$) and strong dilution ($p = 0.5$). The dynamic critical exponent from our non-equilibrium simulation supports distinctly $z \approx 2.18$ as suggested previously, as opposed to the existing larger values.

1. Introduction

The critical properties of many magnetic materials can be described by the Heisenberg model [1]. Nonetheless, the materials tend to magnetize in the direction of quantization introduced by the magnetic field, which leads to a high anisotropy in spin space. The Ising Hamiltonian is proven to be useful in characterizing the anisotropic case [2], thus breaking the $O(3)$ symmetry of the interaction in the Heisenberg Hamiltonian. However, there do not exist entirely pure materials in nature and impurities inevitably appear in real matters. In many situations, the typical time scale of thermal fluctuations in the pure system is clearly distinguished from the time scale of the impurity dynamics, such that to a very good approximation, the frozen nonmagnetic impurities can be treated as uncorrelated quenched randomness [3]. Therefore, the Ising model with the randomness turns into a prototypical model of the real magnetic materials.

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For the three-dimensional (3D) dirty Ising systems, according to Harris criterion [4], a new universality class controlled by the random fixed point is expected because the specific heat critical exponent in the pure version $\alpha_{\text{pure}} = 0.1103 > 0$ [5], which was supported by theoretical and experimental work [6,7]. It is a focus that identifies asymptotic critical exponents at the random fixed point from effective ones in numerical investigations due to the influences of Ising fixed point and possible percolation fixed point. For the 3D site-diluted Ising model (SDIM), the critical exponents from early Monte Carlo (MC) simulations were dilution-dependent [8], which was attributed to the crossover phenomenon that governs a large interval of the critical region [9]. By a proper infinite volume extrapolation with taking into account the leading correction-to-scaling terms, Ballesteros et al. obtained disorder-independent critical exponents $\nu = 0.6837(53), \beta = 0.3546(28), \alpha = -0.051(15), \gamma = 1.342(10)$ with correction exponent $\omega = 0.37(6)$ when spin concentration $p' = 0.4, 0.5, 0.65, 0.8$ whereas the data of $p' = 0.9$ seem to be still crossing over from the pure fixed point to the diluted one [1]. Another solution is to select a particular spin concentration at which the corrections to scaling or crossover effects are suppressed. For instance, when $p' = 0.8$ the consistent critical exponents with $\nu = 0.683(2), \beta = 0.354(1), \alpha = -0.049(6), \gamma = 1.341(1)$ were extracted by the high-statistics MC simulation [10]. However, the short-time dynamics investigation observed that the systems with $p' = 0.95$ and $p' = 0.8$ are characterized by close agreement of the critical exponent values and they belong to the same class of universal critical behavior with the averaged critical exponents $\nu = 0.677(11), \beta = 0.352(5)$, and $\omega = 0.387(60)$ [11]. For the 3D bond-diluted Ising model (BDIM), the studies are relatively few. Berche et al. acquired asymptotic critical exponents $\nu = 0.68(2), \beta = 0.35(1), \gamma = 1.34(1)$ by introducing temperature scaling [12] and exhibited the great influence of the crossover phenomena between the pure, disorder and percolation fixed points, which lead to the dilution-dependent effective critical exponents. From the finite-size scaling analysis it was found that the correction exponent ω vanishes for all quantities at bond concentration $p = 0.54(2)$ with asymptotical critical exponents $\nu = 0.683(2), \eta = 0.036(1)$ [10]. In conclusion, although the asymptotic critical exponents ν and β extracted from different references seem to be consistent, the asymptotic disorder amplitudes located are divergent. Therefore, the analyses on the crossover effects are necessary for further understanding phase transition in dilute magnetic materials. In this paper, we will derive the scaling function characterizing the crossovers in the frame of the finite-time dynamics approach to probe the critical behavior thoroughly.

On the other hand, the universality of the random fixed point with respect to the forms of disorder ($\pm J$, site-, bond-dilution, and random-bond) has been demonstrated [10,12–15]. However, $\gamma = 1.306$ from a nonperturbative approach [16], $\gamma = 1.305(5)$ from a high-temperature series expansion [17], and $\alpha = -0.10(2)$ from an experimental work [18] are slightly smaller than the corresponding critical exponents aforementioned. Furthermore, a numerical work indicated the possible existence of two classes of universal critical behavior for the SDIM with different modes of behavior for weakly and strongly disordered systems [19], which contradicts with the single universality class suggested [1,11,12,15,20].

In contrast to the static exponents, the existing dynamic critical exponents can fall into three categories: $z \approx 2.18$, $z \approx 2.35$, and $z \approx 2.6$. The early experimental investigation obtained $z = 2.18(10)$ [21]. Subsequent renormalization group (RG) with resummation techniques of two- to three-loop dynamical functions gave $z \approx 2.18$ [22], $z = 2.191$ [23], and $z = 2.172$ [24], all of which are close to $z = 2.196(17)$ from short-time dynamics work, in which the dynamic exponents were acquired by fitting Binder cumulant with respect to the MC time in a macroscopic short-time region [11]. However, the analysis of the size-dependence of autocorrelation times at the critical point provides the estimate $z = 2.35(2)$ by equilibrium simulation [25], which is compatible with $z = 2.36(9)$ found in the high-temperature paramagnetic phase [26]. Furthermore, the calculations in the off-equilibrium regime determined the value $z = 2.62(7)$ [27], which is in accordance with $z = 2.6(1)$ from another non-equilibrium simulation [28]. Clearly, further studies for the system are necessary.

Our studies for the 3D random-bond Ising model identified asymptotic critical exponents with $\nu = 0.686(25), \beta = 0.346(8), \alpha = -0.049(24), \gamma = 1.332(31), z = 2.114(51)$ [15] from crossover ones by verifying both the hyperscaling law and the Rushbrooke scaling law and their combined scaling law. Although in coincidence with most existing results within errors, the static exponents should be more accurately measured with smaller errors. Moreover, the dynamic exponents appear to be somewhat smaller compared to $z \approx 2.18$ alluded above.

Motivated by these reasons, this paper will focus on three points by the finite-time dynamics approach within the frame of the 3D BDIM: (i) the semi-quantitative analyses of the crossover effects to further understand the critical behavior by introducing a scaling function, (ii) the improvement in the estimates of critical exponents, particularly, the dynamical exponent, (iii) the further confirmation of the single universality class. Here we shall also show that the Monte Carlo renormalization group (MCRG) calculations applied by the previous work [15,29–31] which take generally a long computer time is not essential. Furthermore, we obtain more accurate asymptotic dynamic exponent $z = 2.170(11)$, supporting unequivocally $z \approx 2.18$ suggested.

2. Model and method

2.1. Model

The Hamiltonian of the 3D BDIM with independent quenched random interactions is

$$H = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j, \tag{1}$$