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Zeros in Partition Function and Critical Behavior of Disordered Three Dimensional Ising Model

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We used a Monte Carlo simulation of the structurally disordered three dimensional Ising model. For the systems with spin concentrations $p = 0.95, 0.8, 0.6$ *and* 0.5 *we calculated the correlation-length critical exponent* ν *by finite-size scaling. Extrapolations to the thermodynamic limit yield* $\nu(0.95) = 0.705(5)$, $\nu(0.8) = 0.711(6)$, $\nu(0.6) = 0.736(6)$ *and* $\nu(0.5) = 0.744(6)$. *The analysis of the results demonstrates the nonuniversality of the critical behavior in the disordered Ising model.*

Keywords: Monte Carlo simulation, complex temperature, critical exponents, disordered systems,zeroes of the partition function.
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The analysis of the effect of the structural disorder on second order phase transitions leads to the following two questions. First, do the critical exponents of a "pure" magnetic system change at the dilution of it by nonmagnetic impurities? Second, if they do change, are these new critical exponents universal, i.e., independent of the concentration of structural effects up to the percolation threshold? The answer to the first question was given in [1]. It was shown that the critical exponents for the systems with quenched structural defects differ from those characteristic of similar systems without defects if the critical exponent for the specific heat in the pure system is positive. This criterion is met only for three dimensional systems with the critical behavior described by the Ising model. The critical behavior of dilute Ising-type magnetic systems was studied in [2–9] using the renormalization-group techniques, numerical Monte Carlo simulations, and experimental methods. Currently, we have a positive answer to the question concerning the existence of the novel universality class for dilute Ising-type magnetic systems. However, it is still not quite clear whether the asymptotic values of the critical exponents are independent of the degree of dilution in the system, how the crossover effects can change these values, and whether two or more regimes of the critical behavior for weakly and strongly disordered systems can exist. These questions are still open and are actively discussed.

1. Model and observables

We consider a model of disordered spin system in the form of a cubic lattice with linear size L under certain boundary conditions. The microscopic Hamiltonian of the disordered Ising model can be written in the form

$$H = -J \sum_{<i,j>} p_i p_j S_i S_j, \qquad (1)$$

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where J is the short-range exchange interaction between spins S_i fixed at the lattice sites and taking on values of ± 1. Nonmagnetic impurity atoms form empty sites. In this case,occupation numbers p_i taking on the value 0 or 1 and are described by the distribution function

$$P(p_i) = (1-p)\delta(p_i) + p\delta(1-p_i), \tag{2}$$

with $p = 1 - c$, where c is the concentration of the impurity atoms. The impurities are uniformly distributed over the entire system, and their positions are fixed in simulation for an individual impurity configuration. We consider here disordered systems with spin concentrations $p = 0.95, 0.80, 0.60$ and 0.50. The partition function of the pure $3D$ Ising model on a lattice of extent L without an applied magnetic field and at an inverse temperature $\beta = 1/T$ in terms of the total energy, E is

$$Z(\beta) = \sum_{S_i} \exp(-\beta E) = \sum_E p(E,\beta)\exp(-\beta E), \tag{3}$$

where $p(E,\beta)$ is the density of states. A complex zero in the partition function indicates a non-analyticity in the free energy. In the thermodynamic limit ($L \to \infty$), the pinching of such zeros of the real temperature axis precipitates a phase transition. Nevertheless we can study the transition in a finite system by analytical continuation to complex temperatures, $\beta = \eta + i\xi$. In this case the partition function includes both oscillating and damping factors[10]:

$$Z(\beta) = \sum_E p(E,\beta)\exp(-(\eta + i\xi)E) = \sum_E p(E,\beta)\exp(-(\eta E)[\cos(\xi E) - i\sin(\xi E)]. \tag{4}$$

By rescaling with $Z[Re(\beta)]$ we define the quantity:

$$R = \frac{Z(\beta)}{Z[Re(\beta)]} = \frac{\sum_E p(E,\beta)\exp(-(\eta + i\xi)E)}{\sum_E p(E,\beta)\exp(-(\eta E)} = <\cos(\xi E)>_\eta - i<\sin(\xi E)>_\eta. \tag{5}$$

Therefore the partition function at complex temperature $\beta = \eta + i\xi$ can be constructed using expectation values taken at real temperatures $\beta = \eta$. The Fisher zero is a complex temperature value (η, ξ) such that $R = 0$. Our objective is to obtain the locations of the Fisher zeros for several system sizes. To achieve this we performed MC simulations in the vicinity of the critical temperature. The crucial point is that we can use histogram techniques [11] to evaluate $<\cos(\xi E)>_\eta$ and $<\sin(\xi E)>_\eta$ near the simulation temperature. With this in hand, we can then minimise R^2 using numerical optimization methods.

2. Simulation details and results

We performed extensive simulations of the model for linear lattice sizes from L = 18 to 32 with periodic boundary conditions. As a time unit, we used Monte Carlo step per spin (MCS) corresponding by 10 Wolf clusters updates. For termolization of system we used 10^6 MCS and $2 \cdot 10^6$ MCS used for averaging. To determine the average values of thermodynamic functions, averaging over various impurity configurations was carried out along with statistical averaging (averaging was carried out over 400 samples). We have performed two set of simulations. Firstly we simulated every lattice size at β_c [5] ($\beta_c(0.95) = 0.2345947(2)$, $\beta_c(0.8) = 0.285757(2)$, $\beta_c(0.6) = 0.412519(3)$ and $\beta_c(0.5) = 0.541979(3)$) as this should be the more direct approach to estimate critical quantities. We can obtain the critical exponent ν by the scaling of the real and imaginary part of the zeros . The scaling of the first zeros is shown on a double-logarithmic scale in Figs. 1, 2.

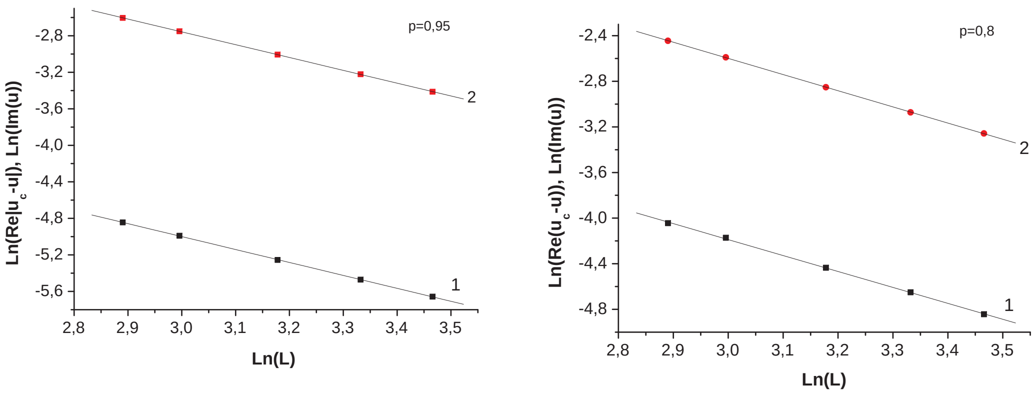

Fig. 1. Scaling of the real part 1 and imaginary 2 of the first Fisher zeros for $p = 0.95$ and $p = 0.8$. In each case the error bars are smaller than the symbols

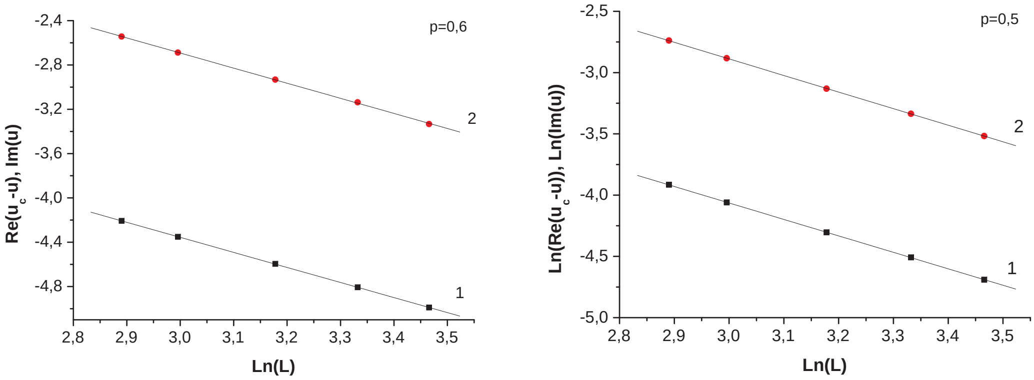

Fig. 2. Scaling of the real part 1 and imaginary 2 of the first Fisher zeros for $p = 0.6$ and $p = 0.5$. In each case the error bars are smaller than the symbols

Therefore we fit each of $Re(u_c - u)$ and $Im(u) \sim aL^{-1/\nu}(1 + bL^{-\omega})$,where ω is the critical exponent for the correction to scaling. The values of ω for different spin densities are taken from [5] $\omega(0.95), \omega(0.8) = 0.23(13)$ and $\omega(0.6), \omega(0.5) = 0.28(15)$. After including this correction to scaling, we obtain the values: $\nu(0.95) = 0.705(5)$, $\nu(0.8) = 0.711(6)$, $\nu(0.6) = 0.736(6)$ and $\nu(0.5) = 0.744(6)$. The results of our investigations lead to the following conclusion. Values of critical exponent for the correlation length demonstrate the existence of two classes of universal critical behavior for the diluted Ising model [4–6] with various characteristics for weakly and strongly disordered systems.

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Нули статистической суммы и критическое поведение неупорядоченной трехмерной модели Изинга

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В статье проведено моделирование методом Монте-Карло критического поведения трехмерной неупорядоченной модели Изинга. Для систем с концентрацией спинов $p = 0.95, 0.8, 0.6$ *и* 0.5*, используя метод конечно-размерного скейлинга для нулей статистической суммы, вычислен критический индекс корелляционной длины* $\nu(0.95) = 0.705(5)$, $\nu(0.8) = 0.711(6)$, $\nu(0.6) = 0.736(6)$ *и* $\nu(0.5) = 0.744(6)$. *Полученные результаты демонстрируют неуниверсальность критического поведения трехмерной неупорядоченной модели Изинга.*

Ключевые слова: метод Монте-Карло, комплексная температура, критические индексы, неупорядоченные системы, нули статистической суммы.