Phase transitions and thermodynamic properties of the antiferromagnetic Potts model on a face-centered cubic lattice

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Abstract. Using the Monte Carlo method we investigate the phase transitions and thermodynamic properties of magnetic structures with non-collinear directions of magnetic moments corresponded to antiferromagnetic q=4 Potts model on a face-centered cubic lattice. Monte Carlo simulations are performed on lattices with linear sizes L=20÷44. Thermodynamic parameters: the order parameter m_{AF}, susceptibility χ, internal energy U, and specific heat C are evaluated for all studied systems. By employing the fourth order Binder cumulant method, a first order transition is shown to be occurred in the model.

1 Introduction

There exists at present a rich body of the experimental material on magnetic substances with crystalline structure and properties of *AnX*-type compounds with the *NaCl* structure. These are so called monopnictides and monochalcogenides, where *An* is a rear-earth element or actinide, *X* is V or VI groups` element (*UN*, *UAs*, *USb*). They display most interesting properties. The evolution of the magnetic neuronography increases a number of experiments in determination of different compound magnetic structures. Rossat-Mignod *et. al.* [1] proved that a single wave vector component is insufficient to describe the experimental data for *UP*, *UAs*, and *USb* compounds. Therefore, multi-**k** structures with wave vectors comprised more than one component (2-**k** structures for two-component wave vector and 3-**k** structures for three-component vector) were proposed. The interpretation of *USb* neuronography is in a better agreement with experimental data of a 3-**k** structure than a collinear model. We notice that this 3-**k** structure corresponds precisely to the q=4 standard Potts model illustrated in Fig. 1.

The investigation of phase transitions (PTs) and thermodynamic properties of the 4-state antiferromagnetic (AF) Potts model is the main goal of this study.

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2 Model and Method

The Hamiltonian of the antiferromagnetic q=4 standard Potts model on a face-centered cubic (FCC) lattice (Fig.1) reads

$$H = -J\sum_{i,j}\cos\theta_{i,j} , \qquad (1)$$

where J is the parameter of antiferromagnetic exchange interaction (J<0), $\theta_{i,j}$ is the angle between interacting spins S_i - S_j. As is evident from Fig. 1, in the model spins occupying lattice sites can orient in hypertetrahedron q-symmetric directions in the dimensionality space q-1 retaining equal angles between any two different directions.

The cubic ferromagnetic q=4 Potts model with nearest neighbor ferromagnetic interactions were studied in works [2, 3]. Authors reported that a second order transition occurred in the models considered.
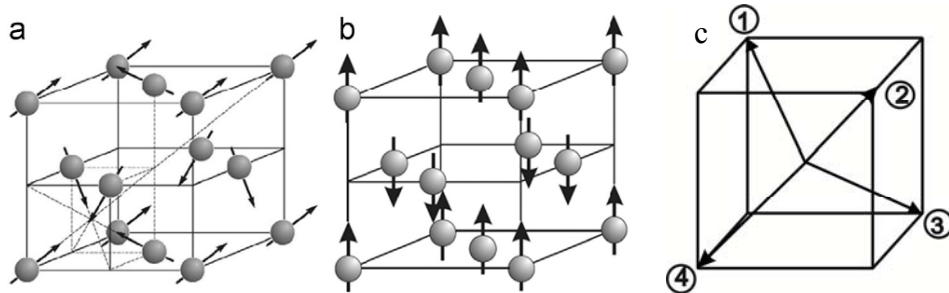

Fig. 1. Identification of the USb diffraction pattern in the 3-k structure (a) and in the collinear one (b). 4-State Potts model (c).

In our study we use the Metropolis algorithm along with the Wolff cluster algorithm [4]. We perform the Monte Carlo simulations for systems of linear sizes 4×(L×L×L) with periodic boundary conditions, where L=28-40. Initial configurations were given so that every spin inside each of sublattices is ordered. To bring the system to equilibrium state the relaxation time τ_0 for all systems with L is computed. Next, the averaging is performed along the Markov chain of length τ=150τ_0 and additional averaging is done by ten different initial spin configurations.

3 Simulation Results

The temperature behavior of the specific heat and susceptibility is evaluated from fluctuation correlations [5]

$$C = (NK^2)(\langle U^2 \rangle - \langle U \rangle^2) , \qquad (2)$$

$$\chi = (NK)(\langle m^2 \rangle - \langle m \rangle^2) , \qquad (3)$$

where K=$|J|/k_B T$, N=4×L^3 is the number of sites, U is the intrinsic energy, m is the order parameter, angle brackets denotes the ensemble average. The order parameter for the antiferromagnetic Potts model is defined as [6]

$$m_{AF} = \left\langle \frac{4}{3}\sum_{\alpha\neq\beta\neq\gamma\neq\varphi}\left(\frac{(N_\alpha + N_\beta + N_\gamma + N_\varphi)}{N} - \frac{1}{4}\right)\right\rangle^{1/2} , \qquad (4)$$

where $N_\alpha = \{N_1, N_2, N_3, N_4\}$, N_1, N_2, N_3, and N_4 are the number of spins in $q=1$, $q=2$, $q=3$, and $q=4$, correspondingly, N_α, N_β, N_γ, N_φ are the number of spins in sublattices *A*, *B*, *C*, and *D*, correspondingly.
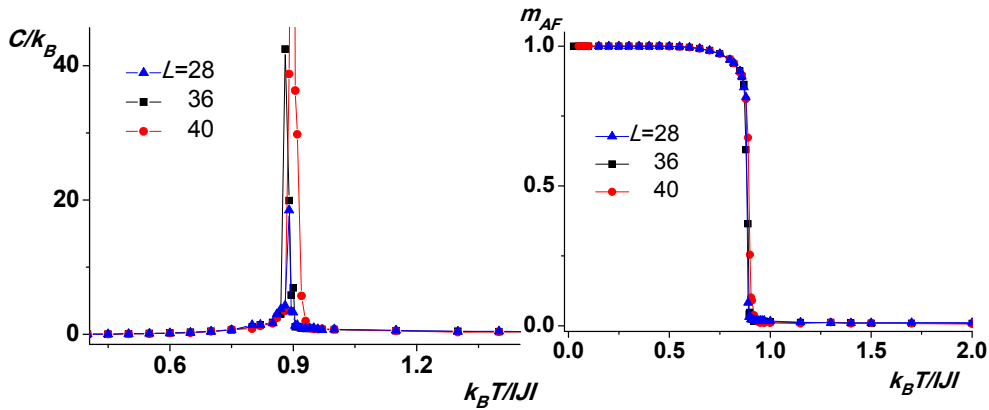

Fig. 2. The temperature dependence of the specific heat *C* for the 3D 4-state Potts model on the FCC lattice.

Fig. 3. The temperature dependence of the order parameter m_{AF} for the 3D 4-state Potts model on the FCC lattice.
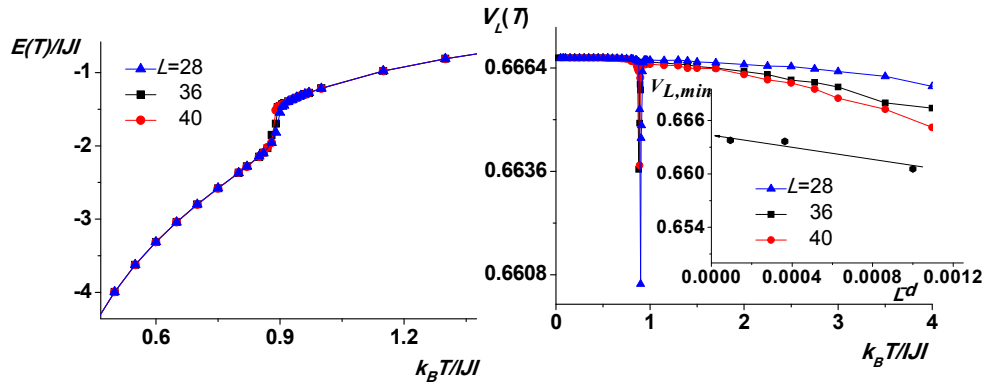

Fig. 4. The temperature dependence of the average energy for the 3D 4-state Potts model on the FCC lattice.

Fig. 5. Dependence of the Binder cumulants $V_L(T)$ on temperature for the 3D 4-state Potts model on the FCC lattice.

Figures 2, 3, 4 and 5 depict the temperature dependences of the specific heat *C*, order parameter m_{AF}, internal energy *E* and Binder cumulants V_L for 3D 4-state antiferromagnetic Potts model on a FCC lattice for systems with *L*=28; 36; 40. From now on an error of data in all figures doesn`t exceed symbol sizes used at plotting the diagrams. As is evident from Figs. 2, 3, and 4, the temperature dependences of the specific heat *C*, order parameter m_{AF}, internal energy *E* for all studied systems exhibit a behavior featured to a first order transition (a jump occurs at PT point). Beyond that, we investigate the dependence of the Binder's cumulants $V_L(T)$ on temperature *T* for this model (Fig. 5). A clearly marked jump at PT point indicates a first order transition. The fourth-order Binder cumulants method [7] has proved to be the most efficient method for the analysis of the character of the phase transition at $T= T_t(L)$.

$$V_L(T) = 1 - \frac{\langle E^4 \rangle_L}{3 \langle E^2 \rangle_L^2}, \tag{5}$$

$$U_L(T) = 1 - \frac{\langle m^4(T,L) \rangle_L}{3 \langle m^2(T,L) \rangle_L^2}, \tag{6}$$

where E is the internal energy and m is the order parameter of the system with L. This technique has proved to be successful for the detection of a PT order, a detail description of that was provided in [8-12]. The averaged value $V_L(T)$ tends to a certain non-trivial value V^* at the first order transition

$$V(T) = V^* + bL^{-d} \tag{7}$$

at $L \rightarrow \infty$ and $T = T_l(L)$, where V^* is distinct from 2/3 at $L \rightarrow \infty$, which is shown in the insert in Fig. 5 for the 3D $q=4$ antiferromagnetic Potts model on a FCC lattice.

Thus, in this study we evaluate within the unified technique the phase transitions and thermodynamic properties of magnetic structures with non-collinear directions of magnetic moments corresponded to the antiferromagnetic $q=4$ Potts model on a FCC lattice. The temperature dependences of thermodynamic parameters for the specific heat C, susceptibility χ, order parameter m_{AF}, and Binder cumulants $V_L(T)$ demonstrate the first order transition. The investigation of the antiferromagnetic $q=4$ Potts model on a FCC lattice permits to elucidate magnetic and thermodynamic properties of real crystals with multi- **k** structures.

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