Thermodynamic and structural properties of systems with SALR interaction on two- and three-dimensional lattices

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Systems with competing interactions are appropriate for modelling biological objects (colloids, ensembles of protein molecules, etc.). The lattice system with attraction between nearest neighbors and repulsion between next-next-nearest neighbors on a square (sq) and simple cubic (sc) lattices is studied.

The competing interactions lead to the order-disorder phase transitions. The geometric order parameter for localizing the phase transition points is introduced for both systems. The critical values 0.655 and 0.186 of the interaction parameter J/k_BT_c for sq and sc lattices respectively were estimated. The phase diagrams of the systems were constructed. The chemical potential sharply changes in the phase transition region, while the thermodynamic factor indicates strong suppressing of fluctuations that is inherent for ordered states of the systems. The complicated behaviour of the correlation functions that reflect structural peculiarities of the system demonstrates an important contribution of competing interactions.

The simple quasi-chemical approximation is proposed for the system under consideration. The concentration versus chemical potential, the thermodynamic factor (the derivative of the concentration logarithm over the chemical potential), and the correlation functions are determined both within the framework of the developed approximate approach and as a result of the Monte Carlo simulation of the lattice system. The proposed analytical approach allows one to correctly describe the qualitative features of the structural properties of systems with competing interactions and can be used to quantify the thermodynamic characteristics of these systems.

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