Thermodynamic equilibrium of large scale Monte Carlo magnetic simulations

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Magnetic simulations take an important place in the area of designing new magnetic materials required for different applications in modern technologies. In this aspect, the Monte Carlo methods are very interesting regarding the fact that they allow modeling complex magnetic systems not only in the basic state but also in realistic temperatures. It is well known that the key point of any applications of the Monte Carlo methods in statistical physics is the condition to keep thermodynamic balance expressed by the Boltzmann probability. Recently, we proposed an original supplementation of the cluster Monte Carlo methods that bases on an configuration entropy of some property (e.g. magnetic anisotropy) [1], which it enhances efficiency for finding minimum of free energy in magnetically multiphase systems. In order to analyze large scale magnetic systems we introduced scaling rules that allow simulating mesoscopic objects by a system with relatively low number of the so-called nodes[2]. This approach requires a redefinition of some parameters occurring in the system Hamiltonian (e.g. exchange integral parameter, spin value, anisotropy constant). The undiscussed problem may arise from the question how is the thermodynamic balance in the "enlarged" systems. The work refers to a set of Monte Carlo magnetic simulations supplemented by the scaling rules. We have tested the ferro-para transition in a function of the scaling factor, i.e., for the systems ranged from nano to meso in size. It turned out that the Curie point had significantly varied with the increasing system size and follows the rule of n^2 (where n is the scaling factor). In the presentation this effect is widely discussed and derived form analysis of the Hamiltonian redefinition proposed as the scaling rules.

References:

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