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Heat capacity of the simple-cubic Ising model

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ABSTRACT

Earlier, the isochoric heat capacity of the cubic lattice for the Ising model was calculated approximately. In the present paper, using the exact solution of the three-dimensional Ising model, this heat capacity is calculated exactly.

KEYWORDS

Ising model;
Heat capacity;
Simple-cubic lattice;
Magnetization;
Partition function;
Nanostructures.

INTRODUCTION

In References[1–4], the specific isochoric heat capacity of the Ising model on the simple-cubic lattice was obtained by approximate methods for various lattice sizes using Monte Carlo simulations. These simulations contain a mistake, because redundant members of the partition function were taken into account in them. In Reference[5], the three-dimensional Ising model was solved exactly and in References[6,7], additional proofs of the correctness of the solution were given. It was shown that there was a flaw in the previous solutions of this model. From the exact solution one can derive the exact expression for the specific heat capacity.

THEORY

Let us consider the one-dimensional uniform Ising model. The nearest-neighbour correlation function for this model is:

$$\Gamma(1) = \tanh(\beta J) \tag{1}$$

where $\beta = 1/kT$, k is the Boltzmann constant, T is temperature, and J is the interaction energy between neighbour spins[5]. Suppose that for β_0 and J_0, $\Gamma(1) = 0.99$. This means that two cases are possible. In the first, about 99% of the spins are turned up and about 1% of them are turned down. In the second, the chain consists of domains and each one contains an average of 50 spins. About half of the domains are turned up, and the rest are turned down. The total magnetisation is zero. Mathematically, the one-dimensional model is solved. Only configurations of these two types may be included in the partition function. The earlier solutions of the one-dimensional problem used the partition function where all possible configurations of the spins were included[5]. This constitutes a mistake, because, for , a configuration with 20% of the spins turned up and 80% of them turned down corresponds to other J and β. For two-, and three-dimensional models one has an analogous situation: earlier solutions included all possible configurations in the partition function, which was a mistake[5].

The partition function of the three-dimensional Ising model in the exact solution is:

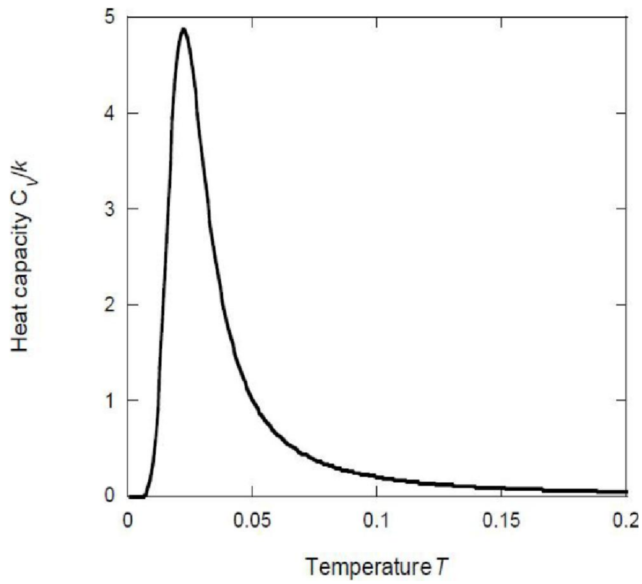

Figure 1 : Isochoric heat capacity C_V / k of the simple-cubic lattice for the Ising model per particle in dimensionless units versus temperature for $J / k = 0.05$ K

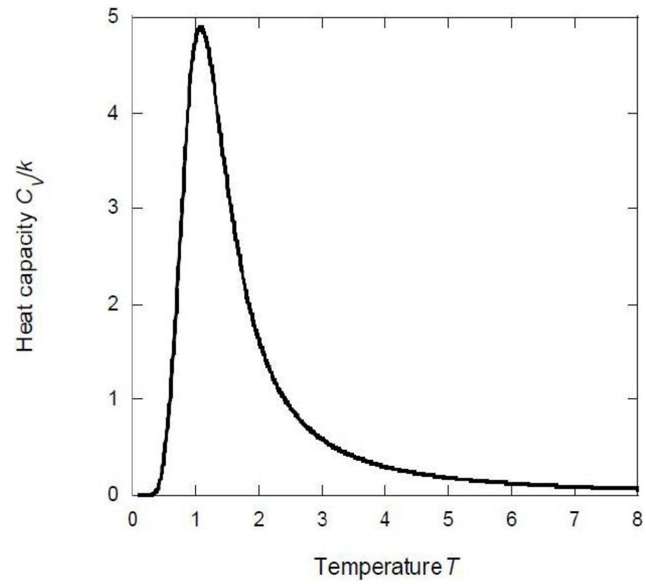

Figure 2 : Isochoric heat capacity C_V / k of the simple-cubic lattice for the Ising model per particle in dimensionless units versus temperature for $J / k = 0.4$ K

$$\mathbf{Z = Z_1 Z_2 Z_3 ...} \quad (2)$$

where Z_i are the partition functions of the elementary cells[5]. According to Reference 5, the exact solution of the Ising model is the exact solution of the elementary cell of the lattice. The partition function of one elementary cell of the simple-cubic lattice in the exact solution is:

$$\mathbf{Z_1 = 4\cosh(3\beta J) + 32\cosh(1.5\beta J) + 60\cosh(\beta J) + 96\cosh(0.5\beta J) + 64} \quad (3)$$

There is one atom per cell in this lattice and therefore, the isochoric heat capacity per atom in this lattice is:

$$\mathbf{C_V = k\beta^2 \partial^2 \ln Z_1 / \partial\beta^2} \quad (4)$$

In dimensionless units, (4) can be expressed as

$$\mathbf{C_V / k = K^2 \partial^2 \ln Z_1 / \partial K^2 = K^2 \left[\frac{\partial^2 Z_1}{\partial K^2} Z_1 - \left(\frac{\partial Z_1}{\partial K} \right)^2 \right] / Z_1^2} \quad (5)$$

where $\mathbf{K = \beta J}$. One can see that the specific heat capacity does not depend on the lattice size, contrary to the results of the previous theories[1–4].

RESULTS AND DISCUSSION

In Reference 1 the following temperatures are considered: $0.3 < T < 4$, and the interaction energy is in the interval $\mathbf{0.15 < \beta J < 0.60}$. That means that $\mathbf{J / k}$ changes approximately from 0.05 to 2.4 K. Equation (5) is solved numerically for both values of $\mathbf{J / k}$ and plotted in Figures 1 and 2. At first glance, it seems that heat capacity must tend to infinity when temperature tends to zero because K tends to infinity. However, one can show that the fraction in (5) tends to zero more quickly in this case. The maximum value of the heat capacities is the same in both figures, and the forms of the curves are similar.

One should mention the paper of Das[8] who tried to solve the one-, two-, and three-dimensional Ising models exactly and to determine the heat capacity. His approach was sound: he understood that magnetisation of the Ising model is that of its elementary cell, but he did not determine the elementary cell of the Ising model correctly.

CONCLUSIONS

Using the exact solution of the three-dimensional Ising model, the specific heat capacity of the simple-cubic Ising model can be calculated very easily. The result differs drastically from those obtained in References[1–4,8] what should be expected. The specific heat capacity does not depend on the lattice size which agrees with experiment and contradicts to the results of the previous theories[1–4].

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