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Baxter–Wu model with fixed magnetization

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Abstract

We study Baxter–Wu triangular model with fixed magnetization in the framework of canonical and microcanonical ensemble, constructing the density of states by Wang–Landau algorithm. We use an approximation similar to a recently developed scheme (critical minimum energy subspace). In this scheme the sampling is not extended to the whole energy spectrum for the given magnetization but it is restricted in a properly determined part of it. We have studied lattices with linear size up to $L = 840$. Our conclusions corroborate analogous conclusions for the square Ising model: An unconventional temperature-driven first-order phase transition take place for lattice sizes above some threshold but this transition ceases to exist at the thermodynamic limit.

Keywords: Ising model; Triangular lattice; Baxter–Wu model; Wang–Landau method

1. Introduction

Ising model with fixed magnetization (IMFM) has recently attracted the interest of the relative research for various reasons. Besides its usefulness for the study of lattice gas, it is the most suitable system for treating a system in the framework of microcanonical ensemble in order to distinguish between a discontinuous and a continuous phase transition on the basis of numerical data obtained for finite systems [1–5].

Thermally driven first-order phase transitions are characterized by a discontinuity in the internal energy and a delta-function singularity in the specific heat. At second-order transitions on the other hand, the discontinuous internal energy becomes continuous with an infinite slope while the specific heat becomes infinite without delta-function singularity but according to a power-law. As it is well known however all these singularities are strictly developed only in the thermodynamic limit. For finite systems in the canonical ensemble these singularities are smeared out and therefore in some cases it is rather difficult not only to distinguish between a first- and a second-order transition but also to conclude if any phase transitions really take place. In order to get round these difficulties many procedures have been proposed, with finite size scaling the more familiar among them. However a different way to study a phase transition is to consider the finite system in the microcanonical ensemble. In this case a first-order transition becomes apparent by a concave intruder in the microcanonical entropy $S(E)$ and a resulting S-shape or backbending in the microcanonical

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caloric curve that means a negative specific heat. The appearance of negative specific heats in small systems is an interesting feature and it is also an experimentally observed fact [6–9].

There are several works concerning Ising model with fixed magnetization using Monte-Carlo simulations [10–14]. In these works the behavior of the model, as we vary the temperature and cross the coexistence line at constant magnetization is investigated. The main conclusion is the existence of a first-order transition but nevertheless for the emergence of this transition a lattice size above some threshold value is needed. Furthermore it is not clear if this first-order transition behavior survives at thermodynamic limit. Pure theoretical considerations on the other hand [15] show that at thermodynamic limit the transition must be continuous.

In the present paper we study the so-called Baxter–Wu model [16–19] as a model of fixed magnetization. We analyze its behavior as we vary temperature keeping the magnetization fixed. Baxter–Wu model is a triangular lattice with Hamiltonian, in the absence of external magnetic field,

$$H = -J \sum_{ijk} s_i s_j s_k, \tag{1}$$

where the sum is taken over all triangles of the lattice and the spins s_i, s_j, s_k take on the values ± 1. This model belongs to the same universality class with the four-state Potts model [20,21] and its more interesting feature is the lack of up–down spin-reversal symmetry of the usual Ising model. The ground state of Baxter–Wu model is four-fold degenerate. There is one ferromagnetic state with all the spins up and three ferrimagnetic states having the spins in one of three sub-lattices up and the spins of the other two down. The magnetization per site for the ferromagnetic state is $+1$ at zero temperature while for the three ferrimagnetic states it is $-\frac{1}{3}$.

For the ferromagnetic state the dependence of the magnetization on temperature has been obtained exactly by Baxter et al. [19] and it is given by

$$m_+ = \left[1 - k^2\left(\frac{ky-1}{y-k}\right)^4\right]^{1/8}, \tag{2}$$

where

$$k = 2\sinh\left(\frac{2J}{k_B T}\right)\operatorname{sech}^2\left(\frac{2J}{k_B T}\right) \tag{3}$$

and y is the solution of the equation

$$\frac{(y-1)^3(1+3y)}{y^3} = \frac{2(1-k^{1/2})^4}{k^{1/2}(1+k)}.$$

A critical temperature is predicted from the above relations at the same point as for a square Ising lattice $k_B T/J = 2/\ln(1+\sqrt{2})$ although the corresponding critical exponents are different. Eq. (2) determines the coexistence curve for the Baxter–Wu model and for positive magnetization. There is also a negative magnetization branch of the coexistence curve not symmetric with the positive one as for the square Ising model. Symmetry considerations and numerical calculations show that this branch is determined by the relation $m_- = -m_+/3$.

The numerical part of the present work consists of the estimation of the density of states $W(E, M)$ for a fixed value of magnetization M by Wang–Landau method. In the following section we review briefly the necessary statistical mechanics and our calculations are presented in Section 3. Finally our conclusions are summarized in Section 4.

2. Theory

In this section we review some concepts of statistical mechanics and we elucidate terms such as micro-canonical and canonical caloric curve or microcanonical and canonical heat capacity.

A microcanonical ensemble for a magnetic system represents a system with fixed energy E and magnetization M. There is a number $W(E, M)$ of configurations or microstates of the system and the