Physica A 509 (2018) 361–368

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Ordered metastable states in the Potts model and their connection with the superheated solid state

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HIGHLIGHTS

- Oscillations between phases in Potts lattices analogous to solid–liquid ones.
- Transition temperature being located at the highest point of the ordered branch.
- Z-method in solids is not a universal behavior of metastable states.
- Correctness of the Z-method cannot be only based on thermodynamical arguments.

ARTICLE INFO

Article history:
Received 26 January 2018
Received in revised form 14 May 2018
Available online xxxx

Keywords:
Potts model
Monte Carlo simulation
Phase transition
Superheating
Spin system
Z-method

ABSTRACT

The superheating effect, in which a solid is heated well above its melting temperature and remains in an ordered, metastable phase, is a well-known phenomenon in materials science. Superheating can be observed experimentally under carefully controlled conditions, and more routinely in atomistic computer simulations. In the context of simulations of superheating, the so-called Z-method is a recently developed technique which allows a precise characterization of the metastable solid state and the melting temperature. However, metastable states are also present in other first-order phase transitions such as the order–disorder transition in spin systems. In spite of all the available work on the behavior of superheated solids, there have been few attempts to characterize the metastable ordered phase in contexts other than melting.

In this work we study the ordered metastable state in a two-dimensional Potts lattice in the microcanonical ensemble under the conditions for first-order transitions. We connect our results with the melting transition in solids, and in particular with the empirical findings of the Z-method. In contrast with the sharp, discontinuous slope of the isochoric curve observed in the melting of solids, an S-shape curve is observed for $T(E)$ in the case of spins. We discuss the implications of our results to extend the Z-method and its applicability for general first-order phase transitions.

1. Introduction

The understanding of first-order phase transitions plays an important role in the statistical physics of finite systems [1] and different phenomena ranging from high-energy physics [2] to materials science [3]. A well-known example is the melting of a solid from a microscopical point of view [4], which often shows a superheated state as a metastable state above the melting temperature. Superheating is a well-studied phenomenon in materials [5–8], manifesting particularly in pristine

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https://doi.org/10.1016/j.physa.2018.06.006
0378-4371/

structures and non-surface solids [9]. The superheating effect has also been observed experimentally [10,11]. Similar to melting, there are ordered metastable states in other first-order phase transitions, for instance in discrete systems [12].

In this work we focus in the order–disorder transition with a "superheated" ordered metastable state [13,14] for a two-dimensional system of Potts spins for different values of the quantity of spin values (q) and a proposed modified Potts model. We compare our results with the Z-method, which is a well-established method to determine the transition temperature of materials by the use of the superheating effect, with the goal of obtaining insights about the particular features of the melting transition that separate it from general first-order phase transitions.

To carry on our study, the main framework is the microcanonical ensemble, where the super-heating is clearly observed. Here microcanonical Monte Carlo simulations are the natural procedure to assess the behavior of spin systems in the superheated regime. We compare the microcanonical results also with results from canonical simulations for the same systems [15,16].

First-order phase transitions allow a clear bridge between the microcanonical and canonical ensembles [15]. In particular, the microcanonical Maxwell construction is equivalent to the equal-peak-height criterion often employed in canonical simulations to determine the transition temperature. This connection is, on the other hand, not directly drawn to the empirical findings of the Z-method [17], which establishes that in microcanonical isochoric simulations there is a maximum energy E_{LS}, corresponding to a temperature T_{LS}, that can be given to crystal before it melts. In practice, this defines the melting temperature as the minimum temperature of the liquid branch of the isochoric (Z) curve. Our results attempt to establish a comparison and unveil the main factors of this discrepancy in first-order phase transitions. As we show in this work, the existence of a kinetic energy term in the Hamiltonian, and the discrete values of Potts spins in the grid, are factors that seem relevant on the differences with the Z-method.

The following section presents the computational procedure and results, giving detailed information of the different simulations, both microcanonical and canonical, under different system sizes and values of q. Section 3 presents some concluding remarks.

2. Computational procedure and results

The Potts model [18] is a generalized Ising model of interacting, "classical" spins q on a regular lattice, which has been used to describe materials [19], biological systems [20,21] and complex networks [22], including social systems [23]. It has also particular importance in QCD [24] and other lines of research in high-energy physics [25].

It is well-established that the Potts model has a first-order phase transition for spin values $q \geq 4$, and a second-order transition for $q < 4$ [26,27]. In this work we will focus on the first-order, order–disorder phase transition. The Potts model consists of spins that are placed on a lattice, with spin values ranged from $s = 1 \ldots q$, and a Hamiltonian given by:

$$H_s = -J \sum_{i,j \neq i} \delta\left(s_i\,, s_j\right), \tag{1}$$

with the sum over all the nearest neighbors pairs, J a coupling constant, which from now on, we will take as equal to 1, and s_x as the spin value (ranged from $1, \ldots, q$) of the x site of the lattice. We will also include a modification of this purely configurational Potts model, in which we introduce an additional kinetic energy term in the Hamiltonian, given by $K = \sum_i \frac{p_i^2}{2m}$.

We use a 2D simulation lattice of $L \times L$ sites with $L = 10$, 20, and 30, with an initial value of $q = 10$. For each case a number of Monte Carlo steps of 3×10^6 have been used.

According to Eq. (1), the energy per spin of the ground state configuration, where every site has the same spin, has a value of -2, and this value is independent of L because of the extensivity of the energy. This is clear if we consider that every site has exactly 4 neighbors, so each site contributes an amount of -4 to the total energy of the lattice, and we divide by 2 to avoid repeated counting.

From this initial, ground state configuration, we evolve each system by a Monte Carlo simulation within the microcanonical ensemble. For this, an additional degree of freedom (a so-called *demon*) is attached to the system. This demon stores and exchanges energy with the system lattice, and it is used as a control parameter to keep the total energy constant [28,29]. At every step of the simulation, if a change that decreases the energy of the lattice is proposed, the change is accepted unconditionally and the energy is incorporated to the demon. If the change increases the energy of the lattice by ΔE, then it is accepted only if the demon has an energy greater or equal to ΔE. After accepting the move, this energy is removed from the demon. Thus, the energy of the full system (lattice + demon) remains constant. As in any genuinely microcanonical simulation, the temperature of the system is not fixed externally, but it is possible to evaluate it from the expression [1]

$$\beta = \log\left(1 + \langle E_d \rangle^{-1}\right), \tag{2}$$

where $\langle E_d \rangle$ is the average value of the demon energy. We performed 3×10^6 steps of simulation keeping the total energy fixed but we discarded the first 1×10^6 equilibration steps to improve the statistical accuracy of the results. Once we have reached equilibrium, we compute the temperature associated with a particular energy, and we increase the energy in steps of 0.04 units per spin, which is the minimum ΔE that we can achieve in a $L = 10$ system. In this manner, we draw the isochoric