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Exact solution of a classical short-range spin model with a phase transition in one dimension: The Potts model with invisible states

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ABSTRACT

We present the exact solution of the 1D classical short-range Potts model with invisible states. Besides the q states of the ordinary Potts model, this possesses r additional states which contribute to the entropy, but not to the interaction energy. We determine the partition function, using the transfer-matrix method, in the general case of two ordering fields: h_1 acting on a visible state and h_2 on an invisible state. We analyse its zeros in the complex-temperature plane in the case that $h_1 = 0$. When $\text{Im}h_2 = 0$ and $r \geq 0$, these zeros accumulate along a line that intersects the real temperature axis at the origin. This corresponds to the usual “phase transition” in a 1D system. However, for $\text{Im}h_2 \neq 0$ or $r < 0$, the line of zeros intersects the positive part of the real temperature axis, which signals the existence of a phase transition at non-zero temperature.

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1. Introduction

Few models in statistical physics can be solved exactly and many of those that can are in a single dimension [1]. Knowing the behaviour of a system in one dimension (1D) can help one to understand and predict its behaviour in higher dimensions too. Also some chemical compounds are effectively described by quasi-1D models [2–6]. For these reasons, 1D models are interesting from both theoretical and experimental points of view.

In the 1920s Wilhelm Lenz and Ernst Ising suggested and investigated the first microscopic model of ferromagnetism [7,8]. Theirs involved a one-dimensional lattice occupied by classical spins which can only be in one of two states: up or down. In the short-range version, only nearest neighbouring spins are allowed to interact. Ising showed that this model has no phase transition at any physically accessible (i.e., non-zero) temperature T [8]. This served as the first and archetypal example of the absence of a finite- T phase transition in 1D classical systems with short-range interactions [9]. Later, in their famous book [10], Landau and Lifshitz gave a heuristic argument that for classical systems there is no phase transition at non-zero temperature in 1D. The approach is based on separately evaluating contributions to the free energy $F = E - TS$ coming from the interaction energy E and the entropy

S . For the Ising model there are two ground states in which all spins are either up or down. At zero temperature the system is in one of these states. At finite temperatures, domain walls separate regions of up- and down-spins. Each domain wall “costs” energy (i.e., it increases the interaction energy E). But in the 1D case this is outweighed by the entropic contribution coming from the number of ways of placing domain walls on the chain. See, e.g., Ref. [11] where it is explicitly shown that adding domain walls reduces the free energy. Therefore, at any temperature it is energetically favourable for domain walls to be inserted. This means the system cannot become ordered and there is no phase transition in such 1D systems.

van Hove proved the absence of a phase transition in one-dimensional fluid-like systems of particles with non-vanishing incompressibility radius and a finite range of forces [12]. This was extended by Ruelle [13] to lattice models. These results are based on the Perron–Frobenius theorem [14]. However, and as emphasised by Cuesta and Sánchez, none of these theorems preclude the existence of thermodynamic phase transitions in general 1D systems with short-range interactions [15]. Indeed Cuesta and Sánchez gave examples of such models and Theodorakopoulos also discussed how the no-go theorems might be circumvented [16]. In Refs. [17,18] the 1D multispin-interaction Ising and Potts models in field are mapped onto corresponding zero-field 2D models with nearest neighbours interactions. Additionally, quantum 1D models offer further examples of systems which can undergo a phase transition at non-zero temperatures because they are related to 2D classical systems [19].

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In the light of these enduring discussions, it is interesting to investigate further circumstances in which classical systems might exhibit a phase transition in 1D. In particular, we are interested in a mechanism in which entropy production can be suppressed in order to sidestep the conditions of the arguments and theorems discussed above. To do so we consider the Potts model with invisible states which was introduced a few years ago [20,21] in order to explain some questions about the order of a phase transition where $Z(3)$ symmetry is broken. It differs from the ordinary Potts model [22,23] by adding non-interacting states; if a spin is in one such state, it is “invisible” to its neighbours. Originally, the corresponding Hamiltonian was written in the form

$$H = - \sum_{\langle i,j \rangle} \delta_{S_i, S_j} \sum_{\alpha=1}^q \delta_{S_i, \alpha} \delta_{S_j, \alpha}, \quad (1)$$

where q and r are the number of visible and invisible states of the Potts variable

$$s_i = 1, \dots, q, q+1, \dots, q+r. \quad (2)$$

The first sum in (1) is taken over all distinct pairs of interacting particles, and the second sum requires both of the interacting spins to be in the same visible state. From now and on we will use the notation (q, r) -state Potts model for model with q visible and r invisible states.

In the ordinary Potts model [22], the parameter $q \geq 2$ has been introduced as an integer denoting the number of (visible) states that a site can be in. However, it has been extended to other values too in order to describe bond percolation ($q = 1$), dilute spin glasses ($q = 1/2$), and gelation ($q = 0$) [23–25]. The parameter q has been extended to complex values as well [26–29]. In a similar way, although an initial interpretation of the parameter r is the number of invisible states, we extend it here to non-integer and even negative values. As we will show below, the latter corresponds to removing entropy from the system and will be key to inducing a phase transition.

Adding invisible states does not change the spectrum of the model, it only changes the degeneracy of energy levels (the number of configurations with a given energy). Even though invisible states do not change the interaction energy, since they change the entropy they affect the free energy. As a consequences, for example, an increase in the number r of invisible states may cause a phase transition to change from second to first order [20,30]. For example the $(2, 30)$ -state model on a square lattice undergoes the first order transition, while the ordinary $(2, 0)$ -state Potts model (i.e. the Ising model) is an iconic example of a continuous transition.

The Potts model with invisible states describes a number of models of physical interest. In particular, the $(1, r)$ -state model can be mapped to the Ising model in a temperature-dependent field [31]. The 1D $(1, r)$ case with nearest-neighbour interactions is equivalent to the Zimm–Bregg model for the helix-coil transition [31]. The multi-spin extension of this model possesses a re-entrant phase transition and is in good agreement with experimental observations for polymer transitions [32,33]. The $(2, r)$ -state Potts model without external fields is equivalent to the Blume–Emery–Griffiths (BEG) model [20,34,35] with a temperature dependent external field. Furthermore, the general q and r case can be interpreted as a diluted Potts model [20,30]

$$H' = - \sum_{\langle i,j \rangle} \delta_{\sigma_i, \sigma_j} (1 - \delta_{\sigma_i, 0}) - T \ln r \sum_i \delta_{\sigma_i, 0}, \quad (3)$$

where $\sigma_i = 0, 1, \dots, q$ is a new spin variable and all invisible states are gathered into one the zeroth state $\sigma_i = 0$.

In this paper we perform an analysis of the partition function zeros to obtain the exact solution for the 1D Potts model with invisible states. In achieving this, we add another exact result to the existing collection of exactly solved models in statistical mechanics. As we will show below, although one-dimensional, the model manifests a transition at non-zero temperature provided some unusual conditions are assumed. We will discuss regimes in which such behaviour is observed and a possible connection with quantum systems.

The rest of the paper is organised as follows: in Section 2 we present the exact solution using the transfer-matrix method, then in Section 3 the existence of a phase transition at non-zero temperature is demonstrated using partition function zeros, and finally conclusions are given in Section 4.

2. Exact solution of the Potts model with invisible states

Let us consider the (q, r) -state Potts model on a chain consisting of N spins with only nearest-neighbour interactions subject to two separate magnetic fields h_1 and h_2 acting on the first visible and the first invisible states respectively. Imposing periodic boundary conditions, the Hamiltonian of such a system may be written as

$$H_{(q,r)} = - \sum_i \sum_{\alpha=1}^q \delta_{S_i, \alpha} \delta_{\alpha, S_{i+1}} - h_1 \sum_i \delta_{S_i, 1} - h_2 \sum_i \delta_{S_i, q+1}, \quad (4)$$

where the sum over i is taken over all sites of the chain.

We will use the transfer matrix formalism [36–38] to obtain the exact solution of the model (4). The Hamiltonian (4) can be expressed as a sum of terms representing one bond each, so that $H_{(q,r)} = \sum_i H_i$ where

$$H_i = - \sum_{\alpha=1}^q \delta_{S_i, \alpha} \delta_{\alpha, S_{i+1}} - h_1 \delta_{S_i, 1} - h_2 \delta_{S_i, q+1}. \quad (5)$$

Then the partition function can be transformed to

$$Z = \sum_s \exp[-\beta H_{(q,r)}] = \sum_s \prod_i \exp(-\beta H_i), \quad (6)$$

where $\beta = 1/kT$ and k is the Boltzmann constant. Now it is easy to define the $(q+r) \times (q+r)$ square transfer matrix with elements

$$T_{ij} = \exp \left[\beta \left(\delta_{S_i, S_j} \sum_{\alpha=1}^q \delta_{S_i, \alpha} + h_1 \delta_{S_i, 1} + h_2 \delta_{S_i, q+1} \right) \right]. \quad (7)$$

Let us denote

$$t = e^{-\beta}, \quad z_1 = e^{\beta h_1}, \quad z_2 = e^{\beta h_2}. \quad (8)$$

With this notation, positive values of temperature T correspond to t ranging from zero to one, and the elements of the transfer matrix can be written in the compact form: $T_{11} = z_1/t$; $T_{ii} = t^{-1}$ for $1 < i \leq q$; $T_{i1} = z_1$; $T_{(q+1)i} = z_2$; and all remaining elements equal to 1.

Based on the transfer-matrix symmetry it is easy to show that it has five different eigenvalues. The eigenvalue $\lambda_0 = 0$ is $(r-1)$ times degenerate because the final r columns of the matrix are proportional. Because $(q-1)$ elements of the main diagonal are equal to t^{-1} , choosing $\lambda = t^{-1} - 1$ one can find $q-2$ linear independent eigenvectors. This reduces the problem to the determination of three more eigenvalues. They can be found using invariant permutations. The above considerations lead to the equation for the three remaining eigenvalues:

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