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Density of states of the *XY* model: An energy landscape approach

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HIGHLIGHTS

- An energy landscape approach is used to study the *XY* model on a square lattice.
- A class of stationary configurations of the Hamiltonian of $O(n)$ models is given by Ising configurations.
- The density of states of a *XY* model is written in terms of that of the Ising model.
- Approximations are proposed and tested to explicitly calculate the density of states.
- The caloric curve and specific heat obtained are in reasonable agreement with simulations.

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ABSTRACT

Among the stationary configurations of the Hamiltonian of a classical $O(n)$ lattice spin model, a class can be identified which is in one-to-one correspondence with all the configurations of an Ising model defined on the same lattice and with the same interactions. Starting from this observation it has been recently proposed that the microcanonical density of states of an $O(n)$ model could be written in terms of the density of states of the corresponding Ising model. Later, it has been shown that a relation of this kind holds exactly for two solvable models, the mean-field and the one-dimensional *XY* model, respectively. We apply the same strategy to derive explicit, albeit approximate, expressions for the density of states of the two-dimensional *XY* model with nearest-neighbor interactions on a square lattice. The caloric curve and the specific heat as a function of the energy density are calculated and compared against simulation data, yielding a good agreement over the entire energy density range.

1. Introduction

A quite recent point of view on the study of the thermodynamic properties of a classical N-body Hamiltonian system, commonly referred to as the "energy landscape" approach [1–4], implies the study of the properties of the graph of the energy function $H : \Gamma_N \to \mathbb{R}$, where Γ_N is the phase space of the system. Examples of applications include disordered systems and glasses [5–7], clusters [1], biomolecules and protein folding [8–10]. In this context a special rôle is played by the stationary points of the energy function. The latter are the points p_c in phase space such that $\nabla H(p_c) = 0$. Based on

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knowledge about the stationary points of the energy function, landscape methods allow to estimate both dynamical and equilibrium properties of a system. In the present paper the attention will be focused only on equilibrium properties.

The natural setting to understand the connection between the stationary points of the Hamiltonian and equilibrium statistical properties is the microcanonical one [11]. This is the statistical description in which the system is considered as isolated; the control parameter is the energy density $\varepsilon = E/N$, and the relevant thermodynamic potential is the entropy density s_N given by

$$s_N(\varepsilon) = \frac{1}{N} \log \omega_N(\varepsilon), \tag{1}$$

where $\omega_N(\varepsilon)$ is the density of states of the system. The density of states is given by

$$\omega_N(\varepsilon) = \int_{\Gamma_N} \mathrm{d}\Gamma_N \delta\left(H - N\varepsilon\right) = \int_{\Gamma_N \cap \Sigma_\varepsilon} \frac{\mathrm{d}\Sigma}{|\nabla H|}, \tag{2}$$

where Σ_ε is the hypersurface of constant energy $N\varepsilon$ and $\mathrm{d}\Sigma$ is the Hausdorff measure; the rightmost integral stems from a co-area formula [12]. When a stationary configuration p_c is considered, the integrand in (2) diverges. In finite-N systems this divergence is compensated by the measure $\mathrm{d}\Sigma$ that shrinks in such a way that the integral in Eq. (2) remains finite. This notwithstanding, the density of states is non-analytic at the corresponding value of the energy density $\varepsilon_c = H(p_c)/N$. Although these nonanalyticities typically disappear in the thermodynamic limit $N \to \infty$, in some special cases they may survive and give rise to equilibrium phase transitions [13–16]. Stationary points of the energy correspond to topology changes in the accessible phase space, and this has suggested a relation between these topology changes and equilibrium phase transitions (see Refs. [17–21] and references therein).

In Ref. [22] an approximate form for the density of states of a paradigmatic class of classical spin models, the $O(n)$ models, was conjectured on the basis of energy landscape considerations. According to the conjecture, the density of states $\omega^{(n)}$ of a classical $O(n)$ spin model on a lattice can be approximated in terms of the density of states $\omega^{(1)}$ of the corresponding Ising model, i.e., an Ising model defined on the same lattice and with the same interactions. The crucial observation is that all the configurations of the corresponding Ising model are stationary configurations of a $O(n)$ model for any n. The density of states would then be given by

$$\omega^{(n)}(\varepsilon) \approx \omega^{(1)}(\varepsilon) g^{(n)}(\varepsilon), \tag{3}$$

where $g^{(n)}(\varepsilon)$ is an unknown function representing the volume of a neighborhood of the Ising configuration in the phase space of the $O(n)$ model. Since the function $g^{(n)}$ comes from the evaluation of local integrals over a neighborhood of the phase space, one expects that it is regular in all the energy density range. Eq. (3) will be discussed in detail in Section 2. The assumptions made in Ref. [22] to derive Eq. (3) are rather crude and uncontrolled. However, were this relation exact, there would be an interesting consequence: the critical energy densities of the phase transitions of all the $O(n)$ models on a given lattice would be the same and equal to that of the corresponding Ising model.

Despite the fact that Eq. (3) is approximate [23] the critical energy densities are indeed, if not equal, very close to each other, whenever a phase transitions is known to take place, at least for ferromagnetic models defined on regular d-dimensional hypercubic lattices. In particular, the critical energy densities are the same and equal to the Ising one for all the $O(n)$ models with long-range interactions, as shown by the exact solution [24], and the same happens for all the $O(n)$ models on an one-dimensional lattice with nearest-neighbor interactions. For what concerns $O(n)$ models with nearest-neighbor interactions defined on (hyper)cubic lattices with $d > 1$, only numerical results are available for the critical energy densities. In $d = 2$ a Berežinskij–Kosterlitz–Thouless (BKT) phase transition is present in the $n = 2$ case, occurring at a value of the energy density that differs of about 2% from the Ising case (see Refs. [22,25] for a deeper discussion [26]). In $d = 3$, the difference between the critical energy densities of the $O(n)$ models and those of the Ising model is smaller than 3% for any n, including the $n = \infty$ case, as recently shown in Ref. [27]. In the most frequently considered cases, that is for $n = 2$ (the XY model), $n = 3$ (the Heisenberg model) and for the $O(4)$ model, it becomes less than 1%.

In two particular cases, where the prediction on the critical energy densities is exact, the derivation of Eq. (3) can be followed rigorously, that is for the mean-field and for the 1d ferromagnetic XY models. In these cases, an expression very similar to Eq. (3), and which reduces to the latter when $\varepsilon \to \varepsilon_c$, can be derived exactly in the thermodynamic limit [25]. The technical aspects of the derivation strongly rely on the peculiarities of the two models and especially on the fact that they are exactly solvable in the microcanonical ensemble. This feature is crucial for the analysis presented in Ref. [25] and its generalization to $O(n)$ models with $n > 2$ in $d > 1$ is unlikely to be feasible.

The aim of the present paper is to show that an approximate expression for the density of states $\omega^{(n)}$ of nearest-neighbor ferromagnetic $O(n)$ models in $d > 1$ can be derived by applying the same energy landscape considerations as discussed above. More precisely, two approximation techniques are presented here: the first one can be seen as the natural generalization of the techniques applied in Ref. [25] for the mean-field and for the 1-d XY models and will be referred to as "first-principle" approximation in the following; the second one will be named "ansatz-based" approximation, its starting point being the ansatz on the form of the density of states given by Eq. (3) supposed to be valid in all the energy density range. These techniques can be applied to estimate the density of states of in principle any $O(n)$ model in $d > 1$. However we have explicitly performed the calculations only for $n = 2$, i.e., for the XY model in $d = 2$; the technical aspects of the generalization to other members of the $O(n)$ class in $d > 2$ will be discussed underway.