Topological transitions in two-dimensional lattice spin models

Silvano Romano*
Unità di Ricerca CNISM e Dipartimento di Fisica "A. Volta," Universitá di Pavia, via A. Bassi 6, I-27100 Pavia, Italy
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A family of classical statistical-mechanical spin models, by now extensively studied in the literature, involves two-component unit vectors, associated with a two-dimensional lattice, with pair potentials restricted to nearest neighbors and possessing $O(2)$ symmetry—i.e., defined by some function of the scalar product between the two interacting spins; these studies often show the existence of a topological phase transition. We show here that, for a wide class of interaction models of the above type, available mathematical results entail the existence of a topological (Berezinskiĭ-Kosterlitz-Thouless-like) transition, as well as a rigorous lower bound on the transition temperature.

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INTRODUCTION

A family of classical statistical-mechanical spin models, by now extensively studied in the literature, involves two-component unit vectors, associated with a two-dimensional lattice, with pair potentials restricted to nearest neighbors and possessing $O(2)$ symmetry—i.e., defined by some function of the scalar product between the two interacting spins; these studies often show the existence of a topological phase transition. The simplest, prototypical case involves a ferromagnetic (odd) interaction proportional to (minus) the scalar product and leads to the well-known Berezinskiĭ-Kosterlitz-Thouless (BKT) transition [1–3]; other functional forms of the interaction, sometimes of different parity, have been studied as well (see, e.g., Refs. [4–6]) and often found to produce a similar topological transition; the even counterparts have been investigated in connection with nematogenic models [6].

The purpose of the present Brief Report is to show that, for a wide class of interaction models of the above type, the available mathematical results entail the existence of a Berezinskiĭ-Kosterlitz-Thouless-like transition, as well as a rigorous lower bound on the transition temperature.

MATHEMATICAL RESULTS

Trigonometric identities involving Legendre polynomials [7] are quoted here for future reference:

$$P_2(\cos\tau) = \frac{1}{4}[3\cos(2\tau)+1], \tag{1}$$

$$P_4(\cos\tau) = \frac{1}{64}[35\cos(4\tau)+20\cos(2\tau)+9]. \tag{2}$$

As for symbols, let us consider a classical planar rotator or *XY* model, consisiting of two-component unit vectors $\mathbf{u}_k$ associated with a D-dimensional (hypercubic) lattice and parametrized by polar angles ϕ_k; let $\mathbf{x}_k$ denote the coordinates of their lattice sites; their interaction potentials are taken to be translationally invariant, restricted to nearest-neighboring pairs of sites and of the general form

$$\Delta = \Delta_{jk} = f(\cos\phi_j, \cos\phi_k, \sin\phi_j, \sin\phi_k), \tag{3}$$

where f is symmetric with respect to the exchange of the two sites j and k, and sufficiently regular, say a continuous function of its arguments (in the following, it will be specialized to a trigonometric polynomial); let m denote an arbitrary positive integer, and let

$$E_m = f(\cos(m\phi_j), \cos(m\phi_k), \sin(m\phi_j), \sin(m\phi_k)), \tag{4}$$

so that $\Delta = E_1$; it has been shown that interaction models defined by the same functional form f but different values of m produce the same partition function, hence the same thermodynamic properties; moreover, their structural properties can be defined in a way independent of m [8,9].

The interaction potential is now taken to have a generalized ferromagnetic polynomial form, isotropic in spin space:

$$\Phi = \epsilon c_0 - \epsilon \sum_{l=1}^{l=M} a_l \cos[l(\phi_j - \phi_k)]; \tag{5}$$

here, ϵ is a positive quantity, setting temperature and energy scale (i.e., $T^* = k_B T/\epsilon$), and all the coupling constants a_l are non-negative, with $a_1 > 0$ and $a_M > 0$. Let A denote the finite set of constants $\{a_l\}$, and let b denote their maximum value; notice also that, by the above mentioned mapping [8,9], an interaction model

$$\Psi_m = \epsilon c_0 - \epsilon \sum_{l=1}^{l=M} a_l \cos[lm(\phi_j - \phi_k)] \tag{6}$$

is equivalent to Φ; the choice $m=2$ defines a nematogenic interaction.

Two special cases of the previous equations (5) and (6) are

$$W_1 = -\epsilon\cos(\phi_j - \phi_k), \tag{7}$$

*Electronic address: Silvano.Romano@pv.infn.it

$$W_2 = -\epsilon P_2[\cos(\phi_j - \phi_k)], \quad (8)$$

which are equivalent to within a temperature rescaling; similarly, an interaction model of the form

$$W_4 = -\epsilon P_4[\cos(\phi_j - \phi_k)] \quad (9)$$

(i.e., within numerical factors, the model studied in Ref. [6]) is equivalent to

$$W_2' = -\frac{5}{64}\epsilon\{4\cos(\phi_j - \phi_k) + 7\cos[2(\phi_j - \phi_k)]\}. \quad (10)$$

Notice also that, by standard trigonometric identities [7], interaction models of the form [4]

$$U_n = -\epsilon \cos^n(\phi_j - \phi_k), \quad n \in \mathbb{N}, \quad n > 2, \quad (11)$$

are special cases of Eqs. (5) and (6) as well.

At sufficiently high temperature (when $D=3$) or possibly at all finite temperatures (when $D=1,2$), the above models produce orientational disorder and the susceptibilty in the disordered region, for a (hypercubic) sample consisting of $V=L^D$ spins, is defined by [10,11]

$$\chi_2 = \frac{1}{V}\beta\langle \mathbf{F}\cdot\mathbf{F}\rangle, \quad \mathbf{F} = \sum_{k=1}^{V}\mathbf{u}_k, \quad \beta = 1/T^*; \quad (12)$$

thus,

$$\chi_2 = \beta\left[1 + (2/V)\sum_{p<q}\Gamma_{pq}\right], \quad \Gamma_{pq} = \langle\cos(\phi_p - \phi_q)\rangle. \quad (13)$$

The Ginibre inequalities [12–14] entail that, at all temperatures,

$$\frac{\partial \Gamma_{pq}}{\partial a_l} \geq 0; \quad (14)$$

i.e., for models defined by Eq. (5) all correlation functions Γ_{pq}, and hence the susceptibility χ_2, are monotonically increasing functions of all positive couplings a_l.

When $D=1,2$, the Mermin-Wagner theorem and its generalizations entail that all models defined by Eq. (5) [or, in more general terms, by a continuous function of the scalar product $\cos(\phi_j-\phi_k)$ [15]] produce no orientational long-range order in the thermodynamic limit and at all finite temperatures; on the other hand, when $D=2$, the model W_1 was rigorously proven to support the BKT transition [16], with an estimated transition temperature $\Theta_1=0.8929$ (see, e.g., Ref. [17]). Therefore, when $D=2$, all models defined by Eq. (5) support a transition to a low-temperature phase whose slow decay of correlations to zero results in infinite susceptibility [this situation is also called quasi-long-range order (QLRO)]; this is a BKT-like transition, which, in turn, can even become a first-order transition, as proven in Refs. [18,19], where references to previous simulation evidence can be found.

Let $\Theta(A)$ now denote the BKT-like transition temperature for the model defined by a given set A of positive coupling constants; then, $\Theta(A)$ is also a monotonically increasing function of all the couplings and the following lower bound holds:

$$\Theta(A) \geq b\Theta_1. \quad (15)$$

For the model investigated by simulation in Ref. [6], the right-hand side of this inequality yields $\frac{35}{55}\Theta_1 \approx 0.56$; the transition temperature estimated there is $\Theta=0.7226$ and satisfies the bound. Transition temperatures were calculated by simulation in Ref. [5] and for models defined by $-1<\delta<0$ [corresponding to $M=2$, $a_1=1$, and $a_2=-\delta/2$, in the notation of Eq. (5)]; they satisfy the corresponding lower bound as well, now defined by $b=1$, and show the expected increase with decreasing δ.

To summarize, available mathematical results define a wider context, with which some recent papers [4–6] can be fruitfully linked.

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