Comment on "Temperature-dependent orientational ordering on a spherical surface modeled with a lattice spin model"

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In Sec. II of the named paper, the authors study the planar model on a regular two-dimensional (square or triangular) lattice and find evidence of an ordering transition at finite temperatures in both cases. It is shown that their findings do not agree with, and appear to ignore, a number of mathematical results, which have been known in the literature for some decades to date, and entail orientational disorder at all finite temperatures, as well as the existence of the Berezinski–Kosterlitz-Thouless transition.

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In Sec. II of the named paper [1], the authors study the planar model on a regular two-dimensional (square or triangular) lattice; they find evidence of an ordering transition at low temperatures in both cases; the reported estimate of the transition temperature for the triangular lattice is $k_B T_c/\epsilon = 1.8 \pm 0.1$, and a value of $k_B T_c/\epsilon \approx 1.2 \pm 0.1$ seems to be implied for the square lattice. This claim invites a few remarks; in order to present our Comment in an appropriate slightly more general setting and to fix notation and ideas, we will be considering here n-component ($n = 2,3$) classical spins (unit vectors) $\boldsymbol{v}_j$, associated with a D-dimensional lattice ($D = 1,2$) and parametrized by appropriate polar or spherical angles; the symbol $\mathbf{u}_j$ will be reserved for the case of two-component unit vectors (as in the paper commented upon), parameterized by the usual polar angles ϕ_j.

Notice that, as for static properties, the interaction potential used in Eq. (1) of the paper commented upon [1] is equivalent [2–4] to its extensively studied magnetic counterpart (with nearest-neighbor interactions), called the plane rotator or the XY model,

$$G_{jk} = -\epsilon \cos(\phi_j - \phi_k), \quad \epsilon > 0; \tag{1}$$

this equivalence also holds for their dynamical behaviors [2,5–7].

I. AVAILABLE MATHEMATICAL RESULTS

Let $D = 1,2$ and $n = 2,3$, and let the pair interaction have the following factorized form:

$$W_{jk} = f(|\mathbf{x}_j - \mathbf{x}_k|)\Phi(\mathbf{v}_j \cdot \mathbf{v}_k), \quad n = 2,3, \tag{2a}$$

where $\mathbf{x}_j$ denotes coordinate vectors of the lattice sites and its angular part possesses rotational $O(n)$ invariance; when $n = 2$ the previous equation can be rewritten as

$$W_{jk} = f(|\mathbf{x}_j - \mathbf{x}_k|)\Phi[\cos(\phi_j - \phi_k)]. \tag{2b}$$

Moreover, let the function f possess finite range, and let Φ be a continuous function of its argument.

Under the stated hypotheses, the Mermin-Wagner theorem and its successive generalizations [8–18] entail that no orientational order can survive at finite temperatures in the thermodynamic (infinite-sample) limit and entail absence of phase transitions at finite temperatures when $D = 1$; in other words, under the above hypotheses,

$$\lim_{N\to+\infty} \mathcal{P}(N,T) = 0, \quad \forall\, T > 0, \tag{3}$$

where N is the sample size (number of particles or spins) and $\mathcal{P}$ denotes the appropriate order parameters; in these cases, molecular field or Landau–de Gennes treatments, predicting an ordering transition at finite temperatures, perform rather poorly, already in qualitative terms.

When $D = n = 2$ and under additional conditions, the existence of the extensively studied Berezinski–Kosterlitz-Thouless (BKT) transition was proven [19]: This is an infinite-order transition to a low-temperature phase possessing no orientational order in the thermodynamic limit but exhibiting slow (inverse-power-law) decay of correlations, which produces infinite susceptbility [4,20–23]; the model defined by the above Eq. (1) is the simplest prototypal case of this behavior.

Estimates of the (inverse) BKT transition temperature for the named model [Eq. (1)] to be found in the literature are $\beta_c = \epsilon/(k_B T_c) = 1.1200 \pm 0.0001$ for the square lattice [24,25] and $\beta_c = 0.6824 \pm 0.0008$ for the less extensively studied triangular one [26,27]. It was also proven [28,29] that in some cases, i.e., for appropriate functional forms of W in Eq. (2b), the transition to the low-temperature phase may turn first order. Finite-size effects in the BKT transition had long been known [30] and were studied in greater detail starting some 20 years ago: It has been shown [31–34] that in this case $\mathcal{P}(N,T)$ decreases so slowly with increasing sample size that the absence of order in the thermodynamic limit becomes compatible with its existence for a finite but *macroscopic* sample, which exhibits a size-dependent pseudotransition temperature, eventually vanishing in the thermodynamic limit.

An additional remark concerns simulation aspects in Ref. [1]: The authors had run calculations with different sample sizes, and their Fig. 1 appears to suggest a consistent decrease in the estimated order parameter with increasing sample size (a finite-size hint of the above results), a point apparently overlooked by them.

II. DATES AND COMPARISONS

The paper commented upon [1] makes comparisons with a previous simulation study [35] (Ref. [16] in the named paper),

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going back to 1980, and basically follows it uncritically. Notice that the authors of Ref. [35] already had some knowledge of the Mermin-Wagner theorem and its extensions (Refs. [6] and [9] in Ref. [35]); they were not aware of the above equivalence between nematogenic and ferromagnetic counterparts (Refs. [2,3] were actually published some years later), but they cautiously pointed out the possibility of finite-size order, very slowly decreasing with increasing sample size. Reference [35] ends with a cautionary comment based on the observation of spin configurations collected in their Fig. 6; the final sentence reads

> "Indeed their observation confirms the view that the two dimensional system does not possess true long–range order, but rather short–range order with a correlation length which increases as the temperature is lowered."

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