New bounds for the critical temperature and the correlation functions of the classical planar rotor

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Spin correlation functions for ferromagnetic plane rotors are shown to decay exponentially or faster with distance at sufficiently high temperatures. Knowing what such temperatures are provides an upper bound on the critical temperature which is in very good agreement with series calculations for three spatial dimensions. For two spatial dimensions, an upper bound on the Kosterlitz-Thouless transition temperature is found which exceeds their estimate by 20%.

In this paper it will be shown that the spin-spin correlation function for classical ferromagnetic planar rotors with nearest-neighbor interactions will be bounded from above by a function which decays exponentially with distance at sufficiently high temperatures. At such "sufficiently high" temperatures there is no long-ranged symmetry-breaking order (by virtue of the Griffith's[1] inequality) and the magnetic susceptibility (the spatial average of the spin-spin correlation function) is finite. The inequality thus provides an upper bound on the critical temperature. For three-dimensional cubic lattices this upper bound turns out to be in good (6%) agreement with high-temperature series calculations. In the limit of infinite spatial dimensionality, when coupled with the Fröhlich, Simon, and Spencer[2] lower bound, it proves that the $d \to \infty$ critical temperature is given by mean-field theory. For two spatial dimensions, the upper bound found here exceeds by 20% the temperature below which Kosterlitz and Thouless[3] estimate (by nonrigorous but strong arguments) that the magnetic susceptibility will be divergent.[4] This is close enough to lend credence to their hypothesis.

Let us consider a lattice with ferromagnetic nearest-neighbor interactions between planar rotors. The Hamiltonian may be written as

$$H = -J \sum_{\vec{r}} \sum_{\vec{a}} \cos(\theta_{\vec{r}+\vec{a}} - \theta_{\vec{r}}) , \tag{1}$$

where $\theta_{\vec{r}}$ denotes the angle of the spin at a site $\vec{r}$ in the lattice, and $\theta_{\vec{r}+\vec{a}}$ the angle at a nearest neighbor of site $\vec{r}$. The number of vectors $\vec{a}$ is half the number of nearest neighbors to a given site. In general the vectors $\vec{a}$ are to be chosen so that each pair of nearest neighbors appears once and only once in (1). For d-dimensional hypercubic lattices $\vec{a}$ would denote the d basis vectors.

We will be interested in $Z_I(n_1, \vec{R}_1; \ldots; n_I, \vec{R}_I)$ defined by

$$Z_I(n_1, \vec{R}_1; n_2, \vec{R}_2; \ldots; n_I, \vec{R}_I) \equiv \prod \int_0^{2\pi} d\theta_r \, e^{-(1/kT)H} \exp\left(i \sum_{1 \le j \le I} \theta_{\vec{R}_j} n_j \right) . \tag{2}$$

Correlations of spins are given by appropriate Z_I divided by Z_0, the partition function. Thus the two-spin correlation function is

$$\langle \vec{S}_{\vec{0}} \cdot S_{\vec{R}} \rangle = R_e [\, Z_2(1, \vec{0}; -1, \vec{R})/Z_0] . \tag{3}$$

Let us exploit the periodicity of the interaction by writing

$$Z_I(\ldots) = \prod_{\vec{r}} \int d\theta_r \left[\prod_{\vec{a}} \sum_{-L \le m_{\vec{r},\vec{a}} \le L} \frac{1}{2L} \exp\left(\frac{J}{kT} \cos(\theta_{\vec{r}+\vec{a}} - \theta_r + 2\pi m_{\vec{r},\vec{a}}) \right) \right] \exp\left(i \sum_j \theta_{\vec{R}_j} n_j \right) . \tag{4}$$

The $m_{\vec{r},\vec{a}}$ are integers ranging from $-L$ to $+L$ for some integer L. Ultimately the $L \to \infty$ limit will be taken. This limit will be taken before letting the number of sites in the lattice pass to infinity. Such an ordering of limits is perfectly reasonable—in real systems the number of sites, while enormous, is still finite. Making use of the Poisson sum formula

$$\sum_{-L \le m \le L} f(m) = \int_{-L}^{L} d\chi f(\chi) \sum_{-\infty < l < \infty} e^{i 2\pi l \chi} \tag{5}$$

for integer l, gives (ignoring multiplicative constants)

$$Z_I(\dots) = \prod_{\vec{r}} \prod_{\vec{a}} \left(\sum_{l_{\vec{r},\vec{a}}} I_{l_{\vec{r},\vec{a}}}(J/kT) \delta_{\sum_a l_{r,a} - l_{r-a,a}, \sum_{1 \le j \le I} n_j \delta_{r,R_j}} \right) \tag{6}$$

in the $L \to \infty$ limit. In (6) $\delta_{A,B}$ is the usual Kronecker symbol

$$\delta_{A,B} = \begin{cases} 0, & A \neq B \\ 1, & A = B \end{cases}$$

and $I_l(x)$ is the modified Bessel function.

$$I_l\left(\frac{J}{kT}\right) \equiv \lim_{L\to\infty} \frac{1}{2L} \int_{-L}^{L} d\chi \, e^{(J/kT)\cos(2\pi\chi)} e^{i2\pi l\chi} = \left(\frac{J}{2kT}\right)^{|l|} \sum_{j=0}^{\infty} \left(\frac{J}{2kT}\right)^{2j} \frac{1}{j!(l+j)!}. \tag{7}$$

Note that, from the power series (7) $I_l(J/kT)$ is positive for positive J (ferromagnetic interactions). In addition, using the power series and the modified Bessel equation, one obtains

$$I_{l+1}(x)I_{l-1}(x) - I_l(x)I_l(x) = \frac{-1}{x} I_l I_{l+1} - \frac{dI_{l+1}}{dx} I_l + I_{l+1} \frac{dI_l}{dx} = -\int_0^x dy \left(\frac{2}{y} I_{l+1}(y) \frac{dI_l(y)}{dy} + \frac{2I_l(y)I_{l+1}(y)}{y^2} \right) \le 0$$

hence, for any integer l,

$$\frac{I_1(x)}{I_0(x)} \ge \frac{I_{|l|+1}(x)}{I_{|l|}(x)}$$

or

$$M_T \frac{I_{|l|}(J/kT)}{I_0(J/kT)} \ge \frac{I_{|l|+1}(J/kT)}{I_0(J/kT)}, \tag{8}$$

where it is useful to define

$$M_T \equiv I_1(J/kT)/I_0(J/kT). \tag{9}$$

The physical motivation underlying the reformulation of Eq. (6) is a generalization of the picture developed by Kosterlitz and Thouless[3] to describe the transition from low to high temperatures in two dimensions. The planar model, (1), in any dimension is characterized by the discreteness of the circulation of spin vortices. At high temperatures the graininess of circulation should not be of any long-ranged importance. Thus differences introduced by replacing the sum, in Eq. (4), over discrete $m_{\vec{r},\vec{a}}$ with the corresponding integral over continuous $\chi_{\vec{r},\vec{a}}$ should not be important in the high-temperature limit. The $l_{\vec{r},\vec{a}}$ measure deviations from the $T \to \infty$ limit due to "quantized" circulation. (The dissipation of flow in a Bose fluid above its λ point is a useful analogy to bear in mind.) Mathematically, of course, Eq. (6) may be obtained by Fourier transforming $\exp(J\cos\theta/kT)$.

All combinations of $\{l_{\vec{r},\vec{a}}\}$ which satisfy the constraints in (6) may be generated by the following graphical method. The partition function Z_0 will be considered first. In this case, one acceptable combination of $l_{\vec{r},\vec{a}}$ is simply that in which all $l_{\vec{r},\vec{a}} = 0$. Let us suppose that $l_{\vec{r}_0,\vec{a}_0}$ for some $\vec{r}_0, \vec{a}_0$ is now increased by unity. This will be denoted by an arrow running from the site $\vec{r}_0$ to $\vec{r}_0 + \vec{a}_0$. Similarly, if $l_{\vec{r}_0,\vec{a}_0}$ is decreased by unity, an arrow running between $\vec{r}_0$ and $\vec{r}_0 + \vec{a}_0$ in the opposite direction is drawn. If l_{r_0,a_0} is to be increased by more than unity from its "vacuum" value of zero then multiple arrows are drawn. The restriction

$$\sum_{\vec{a}} l_{\vec{r},\vec{a}} - l_{\vec{r}-\vec{a},\vec{a}} = \sum_{j \le I} n_j \delta_{\vec{r},\vec{R}_j} \quad \text{for all } \vec{r}$$

means that, when computing the partition function ($I = 0$), the total number of arrows leaving a site is equal to the total number entering it. All permissible configurations of $l_{\vec{r},\vec{a}}$ are therefore generated by considering all possible closed loops on a lattice in which steps are between nearest neighbors. By the number of "steps" in a loop we will refer to the total number of arrows running (in either direction) between nearest neighbors. Permissible configurations include loops in which some nearest-neighbor bonds might be traversed several times, loops which might intersect themselves and configurations in which there are several disconnected loops. In order to avoid overcounting, those loops in which "backtracking" occurs (that is, in which bonds with multiple arrows of opposite sign occur) must be discounted. Thus the loop in Fig. (1a) is discounted because it provides the same configuration of $l_{r,a}$ as that in Fig. (1b). Note that discarding "backtracking" means that each allowed step can only increase the magnitude of an $l_{r,a}$. Formally we write the partition function as

$$Z_0 = I_0\left(\frac{J}{kT}\right)^N \sum C(\mathcal{L}), \tag{10}$$

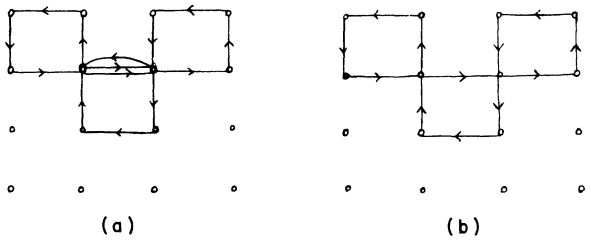

FIG. 1. (a) A loop with "backtracking." This loop is not counted because it prescribes the same configuration of $l_{r,a}$ as the loop in (b). (b) A contribution to the partition function.

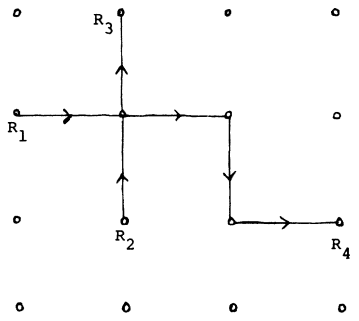

FIG. 2. A contribution to the four-point correlation function Z_4.

where $\mathfrak{L}$ denotes an allowed configuration of loops, N is the number of bonds in the lattice, and

$$C(\mathfrak{L}) \equiv \prod_{\vec{r},\vec{a}} I_{l_{\vec{r},\vec{a}}}\left(\frac{J}{kT}\right) \Big/ I_0\left(\frac{J}{kT}\right) \tag{11}$$

with the $l_{r,a}$ appropriate to the given loop configuration, $\mathfrak{L}$. Note that, by (7), C is positive for ferromagnetic ($J > 0$) interactions.

The considerations of the above paragraph are modified when we wish to deal with spin-spin correlation functions and therefore with the Z_I for $I > 0$. In this case, by (6), there must be a net outflow of n_j arrows from a site R_j. An example of a permissible contribution to $Z_4(1, \vec{R}_1; 1, \vec{R}_2; -1, \vec{R}_3; -1, \vec{R}_4)$ is shown in Fig. 2. Specializing to $Z_2(1, \vec{R}_1; -1, \vec{R}_2)$ we write

$$Z_2(1, R_1; -1, R_2) = I_0\left(\frac{J}{kT}\right)^N \sum_{\mathfrak{L}} \left(\sum_{p_{\mathfrak{L}}} C(p_{\mathfrak{L}}) C(\mathfrak{L}) \right), \tag{12}$$

where $\mathfrak{L}$ denotes any loop configuration used in the partition function and p denotes a path beginning at $\vec{R}_1$, ending at $\vec{R}_2$, and composed of steps between nearest neighbors. To avoid overcounting, $p_{\mathfrak{L}}$ can not intersect any loop in a given configuration $\mathfrak{L}$, of loops. Also to avoid overcounting, $p_{\mathfrak{L}}$, like the loops, must be free of backtracking. The first

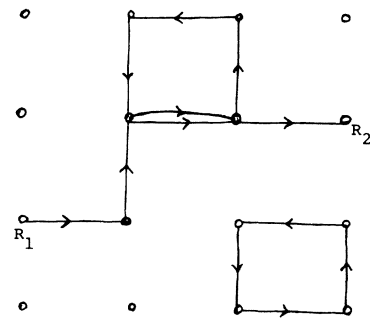

FIG. 3. A contribution to the two-point correlation function Z_2.

restriction on $p_{\mathfrak{L}}$ permits writing the summand in (12) as a product, $C(\mathfrak{L})C(p_{\mathfrak{L}})$. By definition

$$C(p) \equiv \prod_{\vec{r},\vec{a}} I_{l_{\vec{r},\vec{a}}}\left(\frac{J}{kT}\right) \Big/ I_0\left(\frac{J}{kT}\right) \tag{13}$$

with the only nonzero $l_{\vec{r},\vec{a}}$ being those specified by the path p. Thus, for the configuration shown in Fig. 3

$$C(p) = \left(\frac{I_1(J/kT)}{I_0(J/kT)}\right)^6 \left(\frac{I_2(J/kT)}{I_0(J/kT)}\right)$$

and

$$C(\mathfrak{L}) = \left(\frac{I_1(J/kT)}{I_0(J/kT)}\right)^4 .$$

The restriction that no backtracking occur (no bonds have multiple arrows which do not all point in the same direction) means that each time a given bond is traversed in a given path from $\vec{R}_1$ to $\vec{R}_2$ the magnitude of the appropriate $l_{\vec{r},\vec{a}}$ is increased by unity.

Note that any nonbacktracking path, p, may be reexpressed as an appropriate self-avoiding path with superimposed loops. We may choose the self-avoiding path to be such that the superimposed loops do not decrease the magnitude of an l specified by the self-avoiding path. By (8) it follows that the factor, $C(p)$ for the self-avoiding path with superimposed loops is bounded from above by the factor for the self-avoiding path alone: $(M_T)^n$ (where n is the number of steps in the self-avoiding path) multiplied by the C factors for the loops which intersect it. Hence Z_2 is bounded from above by

$$Z_2(1, \vec{R}_1; -1, \vec{R}_2) \leq Z_0 \sum_n \mathfrak{N}_{\vec{R}_1,\vec{R}_2}(n)(M_T)^n , \tag{14}$$

where $\mathfrak{N}_{\vec{R}_1,\vec{R}_2}(n)$ is the number of self avoiding walks with n steps which begin at $\vec{R}_1$ and end at $\vec{R}_2$. Note that there are more loops and paths on the right side of (14) than on the left. Since, for ferromagnetic ($J > 0$) interactions, all C are positive the inequality is not invalidated by overcounting. This upper bound on Z is identical to Domb's[9] "self-avoiding-walk approximation." The upper bound on the critical temperature which is implied by (14) is analogous to a bound obtained, using self-avoiding walks, by Fisher and Sykes[10] for the Ising model.

$$\mathfrak{N}_{\vec{R}_1,\vec{R}_2}(n) \leq \mu^n$$

where $\mu = 4.68$ for simple cubic three-dimensional lattices and 2.64 for square two-dimensional lattices. More careful approximations to $\mathfrak{N}$ are discussed in Domb[9]; they do not lead to an improved bound on the critical temperature and will not be considered here. Applying (14) to (3) we obtain,

for large $\vec{R}$;

$$\langle \vec{S}_{\vec{R}_1} \cdot \vec{S}_{\vec{R}_1+\vec{R}} \rangle \leq \sum_{n_0(\vec{R}) \leq n \leq \infty} \mu^n (M_T)^n , \tag{15}$$

where $n_0(\vec{R})$ is the minimum number of steps possible for a path composed of nearest-neighbor steps which begins at R_1 and ends at $\vec{R}_2 = \vec{R}_1 + \vec{R}$. For large $\vec{R}$,

$$n_0(\vec{R}) \sim |\vec{R}|$$

and, if

$$\mu M_T < 1 , \tag{16}$$

then the spin-spin correlation function has an exponential upper bound:

$$\langle \vec{S}_{\vec{R}_1} \cdot \vec{S}_{\vec{R}_1+\vec{R}} \rangle \leq \frac{\exp\{|\vec{R}| \ln(\mu M_T)\}}{1 - M_T \mu} . \tag{17}$$

One may similarly show that all multiple-spin correlations will fall off exponentially or faster with distance so long as (17) is satisfied. By virtue of the Griffith's inequality

$$\langle \vec{S}_{\vec{R}_1} \cdot \vec{S}_{\vec{R}_2} \rangle \geq \langle \vec{S}_{\vec{R}_1} \rangle \cdot \langle \vec{S}_{\vec{R}_2} \rangle ,$$

there can be no symmetry-breaking long-ranged order so long as (17) is satisfied. Therefore the critical temperature T_c must be such that

$$\mu M_{T_c} \geq 1 . \tag{18}$$

From the power series (7) and the definition (9) of M_T

$$M_T \leq J/2kT$$

Further, for d-dimensional hypercubic lattices

$$\mu \leq 2d - 1 .$$

Thus

$$kT_c \leq J(d - \tfrac{1}{2}) \tag{19}$$

(19), when coupled with the lower bound of Fröhlich, Simon, and Spencer[2] proves that the critical temperature for the $d \to \infty$ ferromagnetic planar rotor is given by mean-field theory.

In three dimensions, (18) may be evaluated numerically to give, for cubic lattices, an upper bound of 76% of the mean-field critical temperature. This exceeds the critical temperature predicted by series expansions[5] by 6%. (18) gives a nonzero upper bound on T_c for two spatial dimensions. This should not be surprising. Although symmetry-breaking order is prohibited for the $d = 2$, XY model at nonzero temperature[6] there is reason to believe that the magnetic susceptibility (the spatial average of $\langle \vec{S}_0 \cdot \vec{S}_R \rangle$) is infinite below a nonzero T_c. (18) provides an upper bound on that temperature. In order to compare this upper bound with the estimated critical temperature of Kosterlitz and Thouless we will consider, not the usual rotor model, (1), but the periodic Gaussian model:

$$e^{-H/kT} = \prod_{\vec{r},\vec{a}} \sum_{m_{\vec{r},\vec{a}}} \exp\left(\frac{-J}{kT} (\theta_{\vec{r}+\vec{a}} - \theta_{\vec{r}} + 2\pi m_{\vec{r},\vec{a}})^2\right) . \tag{20}$$

Villain[7] has shown that this model is equivalent to Kosterlitz and Thouless' spin waves plus vortices approximation to the XY model. For the periodic Gaussian model (18) remains valid with

$$M_T = e^{-kT/4J} . \tag{21}$$

For a square lattice in two dimensions, $\mu = 2.64$ and

$$kT_c \leq 4J \ln(2.64) \tag{22}$$

which exceeds the Kosterlitz-Thouless estimate $kT_c \cong \pi J$ by 20%.

Note that, for the periodic Gaussian model we use, in place of $I_l(J/kT)/I_0(J/kT)$:

$$\exp\left(\frac{-kT}{4J} l^2\right)$$

and the graphs in (10) and (12) generate a high-temperature series in powers of $e^{-kT/4J}$. For the equivalent model developed by Chui and Weeks[8] to describe the roughening transition at interfaces, this expansion is a low-temperature expansion. The temperature and coupling constant in the Chui-Weeks model (denoted by T_r and J_r, respectively) are related to the corresponding quantities for the periodic Gaussian model by

$$kT/4J = J_r/kT_r .$$

Finally it should be noted that, for $d = 2$, the spin-waves-plus-vortices model of Kosterlitz and Thouless may be recovered—exactly for the periodic Gaussian model (21) (as Villain has shown) and in the low-temperature limit for the usual model (1). The procedure for square lattices is as follows. Denote the two $\vec{a}$ vectors by $\vec{a}_1$ and a_2. Define integers $\hat{l}_{\vec{r}}$ by

$$\hat{l}_{\vec{r}} \equiv \sum_{j \geq 0} l_{\vec{r}+j\vec{a}_1,\vec{a}_2} . \tag{23}$$

The maximum value of j is such that $r + \max(j)a_1$ lies on the edge of the lattice. By definition

$$l_{\vec{r},\vec{a}_2} = \hat{l}_{\vec{r}+\vec{a}_1} - \hat{l}_{\vec{r}} . \tag{24}$$

When we are computing the partition function, the constraint (6)

$$\sum_{\vec{a}} l_{\vec{r},\vec{a}} - l_{\vec{r}+\vec{a},\vec{a}} = 0 \quad \text{for all } \vec{r}$$

implies that

$$l_{\vec{r},\vec{a}_1} = \hat{l}_{\vec{r}+\vec{a}_2} - \hat{l}_{\vec{r}} . \tag{25}$$

Replacing $l_{\vec{r},\vec{a}}$ with $\hat{l}_{\vec{r}}$ and then performing the transformation (5) gives, for the planar model (1):

$$\begin{aligned} Z_0 &= \prod_{\vec{r}} \int dx_{\vec{r}}\, I_{x_{\vec{r}+\vec{a}_1} - x_{\vec{r}}}\left(\frac{J}{kT}\right) \\ &\quad \times I_{x_{\vec{r}+\vec{a}_2} - x_{\vec{r}}}\left(\frac{J}{kT}\right) \sum_{\hat{m}_{\vec{r}}} e^{2\pi i x_{\vec{r}} \hat{m}_{\vec{r}}} \\ &= \prod_{\vec{r}} \sum_{\hat{m}_{\vec{r}}} \exp\left(-\sum_{\vec{R},\vec{R}'} \hat{m}_{\vec{R}} \hat{m}_{\vec{R}'} v(\vec{R}-\vec{R}')\right)[1+O(T)] , \end{aligned} \tag{26}$$

where the $m_{\vec{r}}$ are integers and $v(r)$ is logarithmic at large $\vec{r}$

$$v(\vec{r}) = \frac{2\pi^2 J}{kT} \sum_{\vec{q}} \frac{e^{i\vec{q}\cdot\vec{r}}}{Q^2(\vec{q})} , \tag{27}$$

where the $\vec{q}$ lie inside the Brillouin zone and

$$Q^2(\vec{q}) \equiv 4 - 2\cos(\vec{q}\cdot\vec{a}_1) - 2\cos(\vec{q}\cdot\vec{a}_2) . \tag{28}$$

(26) is the lattice analog of the model for vortex-vortex interactions studied by Kosterlitz and Thouless. To any finite order in a low-temperature expansion, the corrections to (26) will not introduce any long-ranged terms other than $O(T)$ fractional corrections to those already present in (26). No long-ranged $(\hat{m})^4$, etc., terms are introduced. The model studied by Kosterlitz and Thouless thus appears to be an appropriate one at low temperature.

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