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INFLUENCE OF LONG RANGE FORCES IN ISOTROPIC TWO-DIMENSIONAL MAGNETISM

by

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It is now well known [1,2,3,4] that long range magnetic order cannot exist at finite temperatures in crystalline spin systems having simultaneously the following characteristics: a) two-dimensionality; b) the interactions are isotropic in spin space; c) the range of the interactions is short. Nevertheless, a phase transition exists, detectable in the thermal behaviour of the susceptibility[2,3,4,5]. In order to achieve a more detailed understanding of these facts, we have recently[4] studied the classical XY-model by eliminating the above (a) and/or (b) restrictions. In this way we obtained long range order at finite temperatures. We pretend to show in this paper that the same result is obtained if restriction (c) is the only one to be eliminated.

Let us suppose a cyclic two-dimensional crystal having identical spins in each one of its N lattice points (labeled by the index $\vec{\ell}$). The unit cell is taken to be a square with side length a. Furthermore we assume that the interactions are given by the classical ferromagnetic XY-model, hence the Hamiltonian may be written as follows:

$$\mathcal{H} = - \sum_{\vec{\ell},\vec{\ell}'} J_{\vec{\ell}\vec{\ell}'} \cos\left(\theta_{\vec{\ell}} - \theta_{\vec{\ell}'}\right)$$

where $J_{\vec{\ell}\vec{\ell}'}$ is the exchange integral between the $\vec{\ell}$ - and $\vec{\ell}'$ - sites, and $\theta_{\vec{\ell}}$ is the angular position of the spin located in the $\vec{\ell}$ - site, whose position (relative to an arbitrary lattice site chosen as origin) will be noted $\vec{R}_{\vec{\ell}}$. At low temperatures ($T \to 0$) this system is relatively well described by the Hamiltonian $\mathcal{H}'$ given below

$$\mathcal{H} \simeq \mathcal{H}' = \frac{1}{2} \sum_{\vec{\ell},\vec{\ell}'} J_{\vec{\ell}\vec{\ell}'} \left(\theta_{\vec{\ell}} - \theta_{\vec{\ell}'}\right)^2$$

where a constant term has been eliminated. With the Fourier-transformation

$$\theta_{\vec{\ell}} = \frac{1}{\sqrt{N}} \sum_{\vec{q}} e^{-i\vec{q}\cdot\vec{R}_{\vec{\ell}}}\, \theta_{\vec{q}}$$

we may re-write

$$\mathcal{H}' = \sum_{\vec{q}} \kappa_{\vec{q}} \left|\theta_{\vec{q}}\right|^2$$

with $$\kappa_{\vec{q}} \equiv \sum_{\vec{\ell}'} J_{\vec{\ell}\vec{\ell}'} \left(1 - \cos \vec{q}\cdot\vec{R}_{\vec{\ell}\vec{\ell}'}\right)$$

where $\vec{R}_{\vec{\ell}\vec{\ell}'} \equiv \vec{R}_{\vec{\ell}'} - \vec{R}_{\vec{\ell}}$ and $\vec{q} \in B \equiv$ two-dimensional Brillouin zone. The asymptotic behaviour of $c_{\vec{q}}$ for $|\vec{q}|a \to 0$ will frequently be given by

$$c_{\vec{q}} \sim A\, q^p \qquad [1]$$

where p is a real number and A depends on the direction of $\vec{q}$. The longest the interaction range is, the smallest p is. In particular, if interactions exist only between a few neighbors, then[4] $p = 2$.

The above considerations were done for the limit $T \to 0$. Now, at any temperature, we shall treat the Hamiltonian $\mathcal{H}$ with a variational method, by using a trial Hamiltonian $\mathcal{H}_0$, given by

$$\mathcal{H}_0 = \sum_{\vec{q}} C_{\vec{q}} \left|\theta_{\vec{q}}\right|^2$$

where $C_{\vec{q}}$ will now depend on temperature. We expect of course that

$$T \to 0 \Rightarrow C_{\vec{q}} \to c_{\vec{q}} \quad \forall \vec{q} \qquad [2]$$

The variational Helmholtz free energy is given by

$$\bar{F} = \langle \mathcal{H} \rangle_0 - TS_0 = \langle \mathcal{H} \rangle_0 - \frac{k_B T}{2} \sum_{\vec{q}} \ln \eta_{\vec{q}}$$

where So is the entropy, $\eta_{\vec{q}} \equiv \langle |\theta_q|^2 \rangle_0$ and $\langle \cdots \rangle_0$ means the canonical mean value associated to $\mathcal{H}_0$. The classical equipartition principle leads to

$$C_{\vec{q}} \quad \eta_{\vec{q}} \quad = \quad \frac{1}{2} \quad k_B T$$

Let us define

$$K^{\pm}_{\vec{\ell}\vec{\ell}'} \equiv \langle \cos(\theta_{\vec{\ell}} \pm \theta_{\vec{\ell}'}) \rangle_0 = \exp - \frac{1}{N} \sum_{\vec{q}} (1 \pm \cos \vec{q} \cdot \vec{R}_{\vec{\ell}\vec{\ell}'}) \, \eta_{\vec{q}}$$

$m \equiv$ order parameter $\equiv \langle \cos \theta_{\vec{\ell}} \rangle_0 = \left(K^{+}_{\vec{\ell}\vec{\ell}'} \, K^{-}_{\vec{\ell}\vec{\ell}'} \right)^{1/4}$

where properties of gaussian probatility laws **have** been used (see, for example, Ref. (4)). We see **immediately** that

$$\langle \mathcal{H} \rangle_0 = -N \sum_{\vec{\ell}'} J_{\vec{\ell}\vec{\ell}'} \, K^{-}_{\vec{\ell}\vec{\ell}'}$$

The minimization condition $\frac{\partial \overline{F}}{\partial \eta_{\vec{q}}} = 0 \quad \forall \vec{q}$, leads to

$$\sum_{\vec{\ell}'} J_{\vec{\ell}\vec{\ell}'} K^{-}_{\vec{\ell}\vec{\ell}'} (1-\cos \vec{q}\cdot\vec{R}_{\vec{\ell}\vec{\ell}'}) = \frac{k_B T}{2\,\eta_{\vec{q}}} = C_{\vec{q}} \qquad [3]$$

hence $$\sum_{\vec{\ell}'} J_{\vec{\ell}\vec{\ell}'} K^{-}_{\vec{\ell}\vec{\ell}'} \ln K^{-}_{\vec{\ell}\vec{\ell}'} = -\frac{k_B T}{2}$$ (sum rule).

We shall verify that $T \to 0$ implies $K^{-}_{\vec{\ell}\vec{\ell}} \to 1$,
hence $C_{\vec{q}} \to c_{\vec{q}}$, which satisfies [2] .

By using the quasi-continuum limit, this is to say

$$\frac{1}{N}\sum_{\vec{q}} \to \frac{a^2}{4\pi^2}\iint_B d\vec{q} \qquad \text{if } N\to\infty,$$

we may write (using [3])

$$K^{\pm}_{\vec{\ell}\vec{\ell}'} = \exp - \frac{a^2 k_B T}{8\pi^2}\iint_B d\vec{q}\, \frac{1 \pm \cos\vec{q}\cdot\vec{R}_{\vec{\ell}\vec{\ell}'}}{\sum_{\vec{\ell}'} J_{\vec{\ell}\vec{\ell}'} K^{-}_{\vec{\ell}\vec{\ell}'}(1-\cos\vec{q}\cdot\vec{R}_{\vec{\ell}\vec{\ell}'})}$$

$$\sim \exp - \frac{a^2 k_B T}{8\pi^2}\iint_B d\vec{q}\, \frac{1 \pm \cos\vec{q}\cdot\vec{R}_{\vec{\ell}\vec{\ell}'}}{\sum_{\vec{\ell}'} J_{\vec{\ell}\vec{\ell}'}(1-\cos\vec{q}\cdot\vec{R}_{\vec{\ell}\vec{\ell}'})}$$

$$\sim \gamma_1 \exp - \frac{a^2 k_B T}{8\pi^2}\iint_B d\vec{q}\, \frac{1 \pm \cos\vec{q}\cdot\vec{R}_{\vec{\ell}\vec{\ell}'}}{A\, q^p}$$

$$\sim \gamma_1 \exp - \frac{a^2 k_B T}{8\pi^2 \bar{A}} \iint_B d\vec{q}\, \frac{1 \pm \cos \vec{q}\cdot \vec{R}_{\vec{\ell}\vec{\ell}'}}{q^p}$$

where we have used [1], γ_1 is a pure number of the order of unity, $\bar{A}$ is a mean value, and the equivalences hold for $T \to 0$ and $|\vec{R}_{\vec{\ell}\vec{\ell}'}|/a \to \infty$.

If $p \geqslant 2$, $K^-_{\vec{\ell}\vec{\ell}'}$ is different from zero (as long as p is inferior to 4), but $K^+_{\vec{\ell}\vec{\ell}'}$ vanishes, hence $m = 0$ (<u>no long range magnetic order at finite temperature if the range of the interactions is short</u>).

Concerning $K^-_{\vec{\ell}\vec{\ell}'}$, let us treat the case $p = 2$ which is the normal situation for short range interactions:

$$K^-_{\vec{\ell}\vec{\ell}'} \sim \gamma_1 \exp - \frac{a^2 k_B T}{8\pi^2 \bar{A}} \iint_B d\vec{q}\, \frac{1 - \cos \vec{q}\cdot \vec{R}_{\vec{\ell}\vec{\ell}'}}{q^2}$$

$$\sim \gamma_2 \exp - \frac{a^2 k_B T}{4\pi \bar{A}} \ln \frac{|\vec{R}_{\vec{\ell}\vec{\ell}'}|}{a}$$

$$= \gamma_2 \left(a / |\vec{R}_{\vec{\ell}\vec{\ell}'}| \right)^{a^2 k_B T / 4\pi \bar{A}}$$

where γ_2 is a pure number of the order of unity. This result proves selfconsistently that $K_{\vec{\ell}\vec{\ell}'} \to 1$ if $T \to 0$.

Before treating the case $p < 2$, let us finish our discussion of the case $p = 2$ by looking at the correlation function $S(\vec{R}_{\vec{\ell}\vec{\ell}'})$ and the susceptibility χ_T. The correlation function is defined by

$$S(\vec{R}_{\vec{\ell}\vec{\ell}'}) \equiv \langle (\cos\theta_{\vec{\ell}} - m)(\cos\theta_{\vec{\ell}'} - m)\rangle_0$$

$$= \langle \cos\theta_{\vec{\ell}} \cos\theta_{\vec{\ell}'}\rangle_0 = \frac{1}{2}\left(K^+_{\vec{\ell}\vec{\ell}'} + K^-_{\vec{\ell}\vec{\ell}'}\right)$$

$$= \frac{1}{2} K^-_{\vec{\ell}\vec{\ell}'} \sim \frac{\gamma_2}{2}\left(a / |\vec{R}_{\vec{\ell}\vec{\ell}'}|\right)^{a^2 k_B T/4\pi \bar{A}}$$

where we have used that $p \geqslant 2$ implies $m = K^+_{\vec{\ell}\vec{\ell}} = 0$, and the equivalence holds for $T \to 0$ and $|\vec{R}_{\vec{\ell}\vec{\ell}'}|/a \to \infty$. This kind of correlation function (power law with temperature-dependent exponent) is typical of certain two-dimensional problems[3,4] and different from the usual one (exponential law involving a temperature-dependent coherence length).

The isothermal susceptibility χ_T for vanishing external magnetic field $\vec{H}$, is defined by

$$\chi_T \equiv \lim_{H\to 0} \left.\frac{\partial m(T,H)}{\partial H}\right|_T \propto \frac{1}{T} \sum_{\vec{\ell}'} S(\vec{R}_{\vec{\ell}\vec{\ell}'})$$

$$\propto \sum_{\vec{\ell}'} \left(a/|\vec{R}_{\vec{\ell}\vec{\ell}'}|\right)^{a^2 k_B T/4\pi \bar{A}}$$

This sum diverges if $a^2 k_B T/4\pi\bar{A} \leqslant 2$, hence the susceptibility diverges if the temperature is inferior to a critical value To, and is expected to be finite if T > To. This is the reason why we can **talk** of a phase transition, in spite of the non existence of long range order.

Let us now see the case $p < \mathbf{2}$ **(long range** interactions). For $T \to o$ and $|\vec{R}_{\vec{\ell}\vec{\ell}'}|/a \to \infty$ we have

$$K^{\pm}_{\vec{\ell}\vec{\ell}'} \sim \exp - \frac{a^2 k_B T}{8\pi^2 \bar{A}} \int_0^{q^*} \frac{q\,dq}{q^p} = \exp - \frac{a^2 k_B T\, q^{*\,2-p}}{8\pi^2 \bar{A}(2-p)}$$

hence

$$m = \left(K^{+}_{\vec{\ell}\vec{\ell}'} K^{-}_{\vec{\ell}\vec{\ell}'}\right)^{1/4} \sim \exp - \frac{DT}{2-p}$$

where $q^* \simeq \pi/a$ and $D \equiv k_B a^2 q^{*\,2-p}/16\pi^2 \bar{A}$.

The thermal behaviour of the order parameter m is represented in the Figure, where we see clearly in which way the long range order desappears in this classical isotropic two-dimensional magnetic system, when the range of the interactions becomes too short **this is to say when $(2-p) \to + 0$.**

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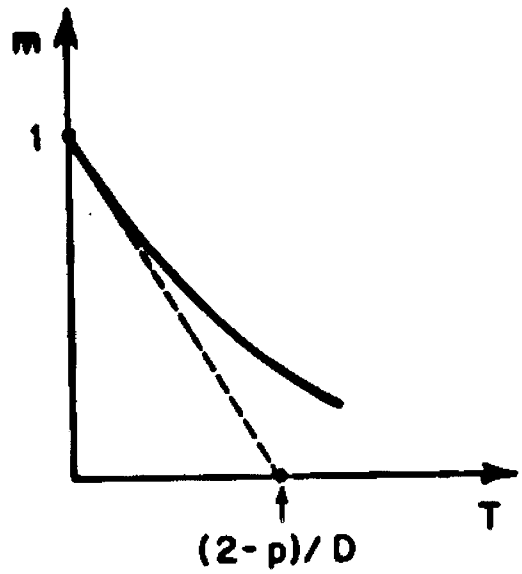
m
1
T
(2-p)/D