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On the spherical model of a ferromagnet

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Abstract

The spherical model of a ferromagnet is briefly reviewed.

The energy of the Ising ferromagnet is given by

$$E = -\frac{1}{2}J\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}\mu_{\mathbf{r}}\mu_{\mathbf{r}'} \quad , \tag{1}$$

where J is a coupling constant and $\mu_{\mathbf{r}} = \pm 1$ are spin variables on lattice sites defined by $\mathbf{r}$. The question would be that of computing the partition function

$$Z = \sum_{\{\mu_{\mathbf{r}}\}}\exp\left(\frac{1}{2}K\sum_{\langle\mathbf{r},\mathbf{r}'\rangle}\mu_{\mathbf{r}}\mu_{\mathbf{r}'}\right) \quad , \tag{2}$$

where the summation extends over all distinct spin configurations and $K = J/T$, T being the temperature. For a one-dimensional lattice the partition function is easily computed by iterating a transfer matrix;[1] for two-dimensional lattices the partition functions have been computed by algebraic methods.[2] The Ising model has no critical point in one dimension, it has one, however, in two dimensions. For three-dimensional lattices the partition function could not have been computed as yet. The spherical model has been introduced[3] as an approximation to the Ising model, and it has been shown that it does not exhibit a critical point in one and two dimensions, but it has one in three dimensions. The spherical model is presented in the following, in a slightly different manner than one usually does.

The Fourier transform of the spin variables

$$\mu_{\mathbf{r}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}}e^{-i\mathbf{kr}}\mu_{\mathbf{k}} \ , \ \ \mu_{\mathbf{k}} = \frac{1}{\sqrt{N}}\sum_{\mathbf{r}}e^{i\mathbf{kr}}\mu_{\mathbf{r}} \ , \ \ \mu^*_{-\mathbf{k}} = \mu_{\mathbf{k}} \quad , \tag{3}$$

where the summation over $\mathbf{k}$ is extended over the first Brillouin zone, allows one to recast the partition function into

$$Z = \sum_{\{\mu_{\mathbf{r}}\}}\exp\left[\frac{1}{2}K\sum_{\mathbf{k}}\varepsilon\left(\mathbf{k}\right)\left|\mu_{\mathbf{k}}\right|^2\right] \quad , \tag{4}$$

where

$$\varepsilon\left(\mathbf{k}\right) = \sum_{\boldsymbol{\delta}}e^{i\mathbf{k}\boldsymbol{\delta}} \quad , \tag{5}$$

$\boldsymbol{\delta}$ being the nearest-neighbours vectors. The Fourier transform $\mu_{\mathbf{k}}$ given by (3) may be viewed as a sum of two scalar products

$$\mu_{\mathbf{k}} = \mathbf{C}(\mathbf{k}) \cdot \boldsymbol{\mu} + i\mathbf{S}(\mathbf{k}) \cdot \boldsymbol{\mu} \quad , \tag{6}$$

where

$$\begin{aligned} \mathbf{C}(\mathbf{k}) &= (\cos \mathbf{kr}_1, \cos \mathbf{kr}_2, ...) \quad , \quad \mathbf{S}(\mathbf{k}) = (\sin \mathbf{kr}_1, \sin \mathbf{kr}_2, ...) \quad , \\ \boldsymbol{\mu} &= \frac{1}{\sqrt{N}} (\mu_{\mathbf{r}_1}, \mu_{\mathbf{r}_2}, ...) \quad , \end{aligned} \tag{7}$$

such that

$$|\mu_{\mathbf{k}}|^2 = C^2(\mathbf{k}) \cos^2 \varphi (\mathbf{k}, \boldsymbol{\mu}) + S^2(\mathbf{k}) \cos^2 \theta (\mathbf{k}, \boldsymbol{\mu}) \quad . \tag{8}$$

The partition function becomes then

$$Z = \sum_{\boldsymbol{\mu}} \exp \left\{ \frac{1}{2} K \sum_{\mathbf{k}} \varepsilon (\mathbf{k}) \left[C^2(\mathbf{k}) \cos^2 \varphi (\mathbf{k}, \boldsymbol{\mu}) + S^2(\mathbf{k}) \cos^2 \theta (\mathbf{k}, \boldsymbol{\mu}) \right] \right\} \quad , \tag{9}$$

with

$$\begin{aligned} C^2(\mathbf{k}) &= \sum_{\mathbf{r}} \cos^2 \mathbf{kr} = \frac{1}{2} N \left(1 + \sum_{\mathbf{s}} \delta_{\mathbf{ks}} \right) \quad , \\ S^2(\mathbf{k}) &= \sum_{\mathbf{r}} \sin^2 \mathbf{kr} = \frac{1}{2} N \left(1 - \sum_{\mathbf{s}} \delta_{\mathbf{ks}} \right) \quad , \end{aligned} \tag{10}$$

$\mathbf{s}$ denoting certain special points in the Brillouin zone. For square and cubic lattices, for example, $\mathbf{s} = 0, \mathbf{s} = \boldsymbol{\pi}$, where $\boldsymbol{\pi}$ stands for $(\pi, \pi, ...)$. The partition function is therefore rewritten as

$$\begin{aligned} Z = & \sum_{\boldsymbol{\mu}} \exp \left\{ \frac{1}{4} KN \sum_{\mathbf{k}}{}' \varepsilon (\mathbf{k}) \left[\cos^2 \varphi (\mathbf{k}, \boldsymbol{\mu}) + \cos^2 \theta (\mathbf{k}, \boldsymbol{\mu}) \right] \right\} \cdot \\ & \cdot \exp \left[\frac{1}{2} KN \sum_{\mathbf{s}} \varepsilon (\mathbf{s}) \cos^2 \varphi (\mathbf{s}, \boldsymbol{\mu}) \right] \quad , \end{aligned} \tag{11}$$

where the prime over summation means all $\mathbf{k}$ except $\mathbf{s}$. It is easy to see that all $\mathbf{C}(\mathbf{k})$ and $\mathbf{S}(\mathbf{k})$ are orthogonal to each other, with $\mathbf{S}(\mathbf{s}) = 0$. One may choose therefore the planes $(\mathbf{C}(\mathbf{k}), \mathbf{S}(\mathbf{k}))$ and $(\mathbf{C}(0), \mathbf{C}(\boldsymbol{\pi}))$ and denote by $\boldsymbol{\rho}(\mathbf{k}, \boldsymbol{\mu})$ the projection of $\boldsymbol{\mu}$ onto the plane $(\mathbf{C}(\mathbf{k}), \mathbf{S}(\mathbf{k}))$ and by $\alpha (\mathbf{k}, \boldsymbol{\mu})$ the angle between $\boldsymbol{\rho}(\mathbf{k}, \boldsymbol{\mu})$ and $\mathbf{C}(\mathbf{k})$, such that

$$\cos \varphi (\mathbf{k}, \boldsymbol{\mu}) = \rho(\mathbf{k}, \boldsymbol{\mu}) \cos \alpha (\mathbf{k}, \boldsymbol{\mu}) \quad , \quad \cos \theta (\mathbf{k}, \boldsymbol{\mu}) = \rho(\mathbf{k}, \boldsymbol{\mu}) \sin \alpha (\mathbf{k}, \boldsymbol{\mu}) \quad ; \tag{12}$$

similarly

$$\cos \varphi (0, \boldsymbol{\mu}) = \rho_s(\boldsymbol{\mu}) \cos \alpha_s (\boldsymbol{\mu}) \quad , \quad \cos \varphi (\boldsymbol{\pi}, \boldsymbol{\mu}) = \rho_s(\boldsymbol{\mu}) \sin \alpha_s (\boldsymbol{\mu}) \tag{13}$$

We note that $\mathbf{C}(0) = (1, 1, ...)$ corresponds to a ferromagnetically ordered $\boldsymbol{\mu}$, while $\mathbf{C}(\boldsymbol{\pi}) = (1, -1, ...)$ corresponds to an antiferromagnetically ordered $\boldsymbol{\mu}$. The partition function may again be rewritten as

$$\begin{aligned} Z = & \sum_{\boldsymbol{\mu}} \exp \left\{ \frac{1}{4} KN \sum_{\mathbf{k}}{}' \varepsilon (\mathbf{k}) \rho^2 (\mathbf{k}, \boldsymbol{\mu}) \right\} \cdot \\ & \cdot \exp \left[\frac{1}{2} KN \varepsilon (0) \rho_s^2 (\boldsymbol{\mu}) \cos 2\alpha_s (\boldsymbol{\mu}) \right] \quad , \end{aligned} \tag{14}$$

where use has been made of $\varepsilon(\boldsymbol{\pi}) = -\varepsilon(0)$.

The spherical model consists in approximating the vectors $\boldsymbol{\mu}$ in (14) on the hypercube with 2^N vortices by a continous variable on a hypersphere of radius unit; obviously, this aproximation is not valid at low temperatures. The spherical approximation amounts to replacing $\alpha(\mathbf{k}, \boldsymbol{\mu})$ by $\alpha(\mathbf{k}) \in (0, 2\pi)$ (and $\alpha_s(\boldsymbol{\mu})$ by $\alpha_s \in (0, 2\pi)$), $\rho(\mathbf{k}, \boldsymbol{\mu})$ by $\rho(\mathbf{k}) \in (0, \infty)$ (and $\rho_s(\boldsymbol{\mu})$ by $\rho_s \in (0, \infty)$), and to replacing the sum in (14) by integration over these continuous variables subject to the condition

$$\sum_{\mathbf{k}}{}'' \rho^2(\mathbf{k}) = \sum_{\mathbf{k}}{}' \rho^2(\mathbf{k}) + \rho_s^2 = 1 \;\; ; \tag{15}$$

since the $\mathbf{k}$'s get correlated by this condition a factor $(N-1)^{N-1}$ should be included in front of the integral, representing how many $\mathbf{k}$'s are counted how many times by integration; in addition, another factor $2^N/\pi^{N-1}$ should also be included, as a consequence of passing from the summation to the integration. The partition function becomes now

$$\begin{aligned} Z &= 2\left(\frac{2}{\pi}\right)^{N-1} (N-1)^{N-1} \prod_{\mathbf{k}}{}' \left[\int_0^\infty d\rho(\mathbf{k}) \cdot \rho(\mathbf{k}) \cdot \int_0^{2\pi} d\alpha(\mathbf{k})\right] \cdot \\ &\cdot \delta\left(\sum_{\mathbf{k}}{}'' \rho^2(\mathbf{k}) - 1\right) \cdot \exp\left\{\frac{1}{4} KN \sum_{\mathbf{k}}{}' \varepsilon(\mathbf{k}) \rho^2(\mathbf{k})\right\} \cdot \\ &\cdot \int_0^\infty d\rho_s \cdot \rho_s \cdot \int_0^{2\pi} d\alpha_s \cdot \exp\left[\frac{1}{2} KN\varepsilon(0) \rho_s^2 \cos 2\alpha_s\right] \;\; . \end{aligned} \tag{16}$$

Introducing $r_{\mathbf{k}} = \rho^2(\mathbf{k}), r_s = \rho_s^2$,

$$I(r_s) = \frac{1}{2\pi} \int_0^{2\pi} d\alpha_s \cdot \exp\left[\frac{1}{2} KN\varepsilon(0) r_s \cos 2\alpha_s\right] \quad , \tag{17}$$

and the Fourier representation of the δ-function one obtains

$$\begin{aligned} Z &= 2^N (N-1)^{N-1} \frac{2}{(2\pi)^2} \int_{-1}^{1} du \frac{1}{\sqrt{1-u^2}} \int d\omega \cdot e^{i\omega} \cdot \\ &\cdot \prod_{\mathbf{k}}{}' \int_0^\infty dr_{\mathbf{k}} \exp\left\{\left[\frac{1}{4} KN\varepsilon(\mathbf{k}) - i\omega\right] r_{\mathbf{k}}\right\} \cdot \\ &\cdot \int_0^\infty dr_s \exp\left\{\left[\frac{1}{2} KN\varepsilon(0) u - i\omega\right] r_s\right\} \;\; . \end{aligned} \tag{18}$$

We introduce now the notations $z_{\mathbf{k}} = \frac{1}{4} K\varepsilon(\mathbf{k}), z_s = \frac{1}{2} K\varepsilon(0)$, perform the integration[4] over $r_{\mathbf{k}}$ and r_s,

$$\int_0^\infty dr_{\mathbf{k}} \exp\{[Nz_{\mathbf{k}} - i\omega] r_{\mathbf{k}}\} = -\frac{1}{Nz_{\mathbf{k}} - i\omega} \quad , \tag{19}$$

introduce also $\omega = -iz$, and get finally

$$\begin{aligned} Z &= 2^N (N-1)^{N-1} \frac{i(-1)^N}{(2\pi)^2} \cdot 2 \cdot \int_{-1}^{1} du \frac{1}{\sqrt{1-u^2}} \int dz \cdot e^z \cdot \\ &\cdot \prod_{\mathbf{k}}{}' \frac{1}{Nz_{\mathbf{k}} - z} \frac{1}{Nz_s u - z} \;\; . \end{aligned} \tag{20}$$

The integration over z, written as

$$\int dz \cdot e^z \cdot {\prod_{\mathbf{k}}}' \frac{1}{Nz_{\mathbf{k}} - z} \frac{1}{Nz_s u - z} = \int dz \cdot e^{\Phi(z)} \quad , \tag{21}$$

where

$$\Phi(z) = z - {\sum_{\mathbf{k}}}' \ln\left(Nz_{\mathbf{k}} - z\right) - \ln\left(Nz_s u - z\right) \quad , \tag{22}$$

is performed by steepest descent; one obtains straightforwardly (for large z)

$$\int dz \cdot e^{\Phi(z)} \cong i\sqrt{2\pi N} z \cdot e^{\Phi(z)} \quad , \tag{23}$$

where z is given by

$$\frac{1}{N} \sum_{\mathbf{k}} \frac{1}{z - z_{\mathbf{k}}} = 1 \ ; \tag{24}$$

the term corresponding to z_s in (22) is irrelevant for z. The partition function can be written now as

$$\begin{aligned} Z \ = \ & 2^N (N-1)^{N-1} \frac{(-1)^{N-1}}{(2\pi)^2} \cdot 2 \cdot \sqrt{2\pi N} \cdot z \frac{e^{Nz}}{N^{N-1}} \cdot \\ & \cdot {\prod_{\mathbf{k}}}' \frac{1}{z_{\mathbf{k}} - z} \cdot \int_{-1}^{1} du \frac{1}{\sqrt{1-u^2}} \cdot \frac{1}{z_s u - z} \quad ; \end{aligned} \tag{25}$$

the integral over u (practically irrelevant) can be approximated by $-\pi/z$ (for large z), so that one obtains

$$Z = 2^N (N-1)^{N-1} \frac{(-1)^N}{\sqrt{2\pi}} \sqrt{N} \frac{e^{Nz}}{N^{N-1}} {\prod_{\mathbf{k}}}' \frac{1}{z_{\mathbf{k}} - z} \quad , \tag{26}$$

or, keeping only the relevant factors,[5]

$$Z = 2^N e^{Nz} \prod_{\mathbf{k}} \frac{1}{z - z_{\mathbf{k}}} \quad . \tag{27}$$

The free energy is therefore given by

$$F = -T \ln Z = -NT \ln 2 - NTz + T \sum_{\mathbf{k}} \ln\left[z - \frac{1}{4} K\varepsilon(\mathbf{k})\right] \quad . \tag{28}$$

and a critical point would appear from the vanishing of the logarithm argument (at least).

Since $\varepsilon(\mathbf{k}) < \varepsilon(0)$ the critical point can only appear for $z = \frac{1}{4}K\varepsilon(0)$. Replacing the sum in (24) by an integral one can see that the integral is singular in one and two dimensions, so that (24) can be fulfilled for $z \neq \frac{1}{4}K\varepsilon(0)$. On the contrary, in three dimensions the integral is finite, so that there is a certain value K_0 above which (24) is no longer satisfied; the term corresponding to $\mathbf{k} = 0$ has to be kept therefore in the summation, and it is precisely this term which ensures the fulfilment of (24). Consequently, in three dimensions there exists a critical temperature T_0 corresponding to K_0, a situation entirely similar to that encountered in the Bose-Einstein condensation.

We specialize now to a simple cubic lattice, and approximate the energy $\varepsilon(\mathbf{k}) = 2\left(\cos k_1 + \cos k_2 + \cos k_3\right)$ by $\varepsilon(\mathbf{k}) = 6 - k^2$; introducing $x = z - z_0 = z - 3K/2$ we can write (24) as

$$N = \frac{1}{x} + \frac{N}{2\pi^2} \int_0^{k_D} dk \cdot k^2 \frac{1}{x + Kk^2/4} \quad , \tag{29}$$

where $k_D = (6\pi^2)^{1/3}$. The critical K_0 is given by

$$N = \frac{2N}{\pi^2 K} \int_0^{k_D} dk \quad , \tag{30}$$

i.e. $K_0 = 2(6/\pi)^{1/3}/\pi$, and the integral in (29) is easily performed. Equation (29) gives $x = 0$ for $K \geq K_0$ and $x = (\pi/2)^2 K_0^3 (1 - K/K_0)^2$ for K slightly below K_0. The energy $E = -J\,(\partial \ln Z/\partial K)$ can now be computed easily. It is continuous at T_0, and the heat capacity is also continuous at this temperature. However, there is a discontinuity in the temperature slope of the heat capacity at T_0, namely

$$c'(T_0^-) = 0, \;\; c'(T_0^+) = -\left[2 + (2/\pi)\,(6/\pi)^{1/3}\left(3\pi^2 - 1/2\right)\right](N/T_0) \quad . \tag{31}$$

One can say, therefore, that the phase transition is of the third order, according to Ehrenfest's classification. The magnetization[5] is infinite for $T \leq T_0$, and goes like $(T - T_0)^{-2}$ above T_0. As one can see the fluctuations in the magnetization are divergent at the critical point.

References

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[2] L. Onsager, Phys. Rev. **65** 117 (1944); see also C. Domb in *Phase Transitions and Critical Phenomena*, ed. by C. Domb and M. S. Green, Academic (1974), vol.3, p.357.

[3] T. H. Berlin and M. Kac, Phys. Rev. **86** 821 (1952); see also G. S. Joyce in *Phase Transitions and Critical Phenomena*, ed. by C. Domb and M. S. Green, Academic (1974), vol.2, p.375.

[4] The integration over $r_{\mathbf{k}}$ can be performed to some upper cut-off with, practically, the same result, for the present discussion, as that given by (19); note that it is this integration by which the singularities appear in the partition function.

[5] In the presence of a magnetic field H an additional factor $\exp\left\{C^2 N/4\left[z - \frac{1}{4}K\varepsilon(0)\right]\right\}$ appears in the partition function, where $C = mH/T$, m being the magnetic moment of the spin; note that the magnetization is given by $M = m\,(\partial \ln Z/\partial C)$ (and the energy is $E = -MH - J\,(\partial \ln Z/\partial K)$).