SPHERICAL ISING MODEL WITH TEMPERATURE-DEPENDENT COUPLING

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The problem of the evaluation of the critical-point exponents is certainly one of the most interesting problems of statistical mechanics. The theoretical effort is mainly concentrated on the series expansion method and the sio-called ε-expansion.

Recently Krizan (1973) suggested to consider the problem of the critical-point exponents of an Ising model within the framework of molecular field theory. On a phenomenological basis a temperature-dependent term is added to the usual Ising Hamiltonian. An example of temperature-dependent interaction is the Debye-Hückel potential in the theory of electrolyte solutions.

The Hamiltonian introduced by Krizan is given by

$$H = -\sum_{n.\,n.} s_i\, s_j - \varepsilon' \sum_i s_i \tag{1}$$

where s_i is the spin on the lattice site i, J is the exchange integral ($J > 0$) between the nearest neighbours on the lattice and ε' is the temperature-dependent coupling. It is defined by

$$\varepsilon' = \begin{cases} c\, k_B\, T_c\, t^p & T \leqslant T_c \\ 0 & T > T_c \end{cases} \tag{2}$$

where c is a constant, k_B is the Boltzmann constant, T_c is the critical temperature, p is a parameter and $t = 1 - T/T_c$. Krizan finds the critical-point exponents from the molecular field theory as functions of p, which is then selected in such a way that the Rushbrooke relation (Stanley, 1971) holds as an equality, namely

$$\alpha' + 2\,\beta + \gamma' = 2. \tag{3}$$

In this manner the following critical-point exponents are obtained $\alpha' = 1/3$, $\beta = 1/3$ and $\gamma' = 1$ while the parameter p is set equal to 1. These critical-point exponents differ from the results of the classical theories. However, although they satisfy (3), they are not in agreement with another result of the scaling hypothesis, namely $\gamma' \neq \beta\,(\delta - 1)$, where $\delta = 3$ in the mean field theory.

In the following we introduce a temperature-dependent coupling of the form (2) in the spherical model of a ferromagnet (Berlin and Kac, 1952). The constraint on the spin variables is given by

$$\sum_{i=1}^{N} s_i^2 = N \tag{4}$$

where N is the number of lattice sites. If an external field B is applied, we should add a term

$$- m B \sum_{i=1}^{N} s_i \tag{5}$$

to the Hamiltonian (1).

The spherical model has been solved exactly by Berlin and Kac and it shows a phase transition in three dimensions, in the absence of an external field. The temperature-dependent interaction ε' will not destroy the phase transition because it is identically equal to zero above the critical temperature.

The Helmholtz free energy found by Berlin and Kac is given by

$$F = - k_B T \left\{ - \frac{1}{2} - \frac{\ln (4K)}{2} + 2 K z_s - \frac{f_3(z_s)}{2} + \frac{(mB + \varepsilon')^2}{(2k_B T)^2\, 2K(z_s - 3)} \right\} \tag{6}$$

where $K = \dfrac{J}{2\, k_s T}$ and

$$f_3 (z) = \frac{1}{(2\pi)^3} \int\!\!\int\!\!\int_0^{2\pi} d\omega_1\, d\omega_2\, d\omega_3 \ln \left[z - \sum_{i=1}^{3} \cos \omega_i \right]. \tag{7}$$

The parameter z_s is the saddle point of the steepest descent evaluation of the partition function. It is given by the solution of

$$4K = \left. \frac{df_3(z)}{dz} \right|_{z=z_s} + \frac{(m B + \varepsilon')^2}{(2 k_B T)^2 K (z_s - 3)^2} \tag{8}$$

Knowing the Helmholtz free energy we can obtain the magnetization

$$M(T) = - \left(\frac{\partial F}{\partial B} \right)_{B=0} = \frac{m\varepsilon'}{2 J (z - 3)}, \tag{9}$$

the isothermal susceptibility

$$\chi(T) = \left(\frac{\partial M}{\partial B}\right)_{B=0} = \frac{m^2}{2J(z_s - 3)} \tag{10}$$

and the specific heat

$$c_M = -T\left(\frac{\partial^2 F}{\partial T^2}\right)_{B=0} = \frac{k_B}{2} - k_B T \left.\frac{\partial f_3}{\partial z}\right|_{z=z_s} \cdot \frac{\partial z_s}{\partial T} +$$

$$+\left[\frac{T\varepsilon'^2}{2J(z_s-3)} - \frac{k_B T^2}{2}\left.\frac{\partial^2 f_3}{\partial z^2}\right|_{z=z_s}\right]\left(\frac{\partial z_s}{\partial T}\right)^2 - \frac{T\varepsilon'}{J(z_s-3)^2}\cdot\frac{\partial z_s}{\partial T}\cdot\frac{\partial \varepsilon'}{\partial T} +$$

$$+\frac{T}{2J(z_s-3)}\left(\frac{\partial \varepsilon'}{\partial T}\right)^2 + \frac{T\varepsilon'}{2J(z_s-3)}\frac{\partial^2 \varepsilon'}{\partial T^2} \tag{11}$$

The results (9—11) are obtained using the definitions of M, χ, c_M and the equation (8) which is satisfied by z_s.

To obtain the critical-point exponents we need to know the behaviour of z_s as a function of t when the critical point is approached. It is easy to see, graphically analyzing (8) that when $t \to 0$, the solution $z_s \to 3$. Because we are interested in the region close to the critical point, we shall solve (8) approximately in the limit $t \to 0$. Hence, we represent the solution of (8) in the form

$$z_s = 3 + A\, t^x \,[1 + 0\,(t^y)] \tag{12}$$

where A, x, y are constants to be determined.

In the region close to the critical point ($z_s \to 3$) the following expansion of $f_3(z)$ derived by Berlin and Kac (1952) is applicable

$$f_3(z) = f_3(3) + 4K_c(z-3) - \frac{\sqrt{2}}{3\pi}(z-3)^{3/2} + O((z-3)^2) \tag{13}$$

where $K_c = \dfrac{J}{2k_B T_c}$.

Using this expansion and substituting (12) and (2) in (8) we obtain the following equation ($B = 0$)

$$4t(z_s-3)^2 = \left(\frac{c\,k_B T_c}{J}\right)^2 t^{2p} - \frac{\sqrt{2}\,k_B T_c(1-t)}{\pi J}(z_s-3)^{5/2} + O((z_s-3)^3). \tag{14}$$

The type of the solution of (14) is a function of the parameter p. A quite straightforward analysis leads to the following result

$$z_s = \begin{cases} 3 + A_1 t^{\frac{4p}{5}}\left[1 + 0\left(t^{\frac{2p}{5}}\right)\right] & 0 < p \leqslant \frac{5}{4} \\ 3 + A_1 t^{\frac{4p}{5}}\left[1 + 0\left(t^{1-\frac{2p}{5}}\right)\right] & \frac{5}{4} < p < \frac{5}{2} \\ 3 + A_2 t^2 \, [1 + 0\,(t)] & p = \frac{5}{2} \\ 3 + A_3 t^{p-\frac{1}{2}}\left[1 + 0\left(t^{\frac{p}{2}-\frac{5}{4}}\right)\right] & \frac{5}{2} < p \end{cases} \tag{15}$$

where

$$A_1 = \left(\frac{\pi c^2 k_B T_c}{\sqrt{2} J}\right)^{2/5}; \quad A_3 = \frac{c k_B T_c}{2J}$$

and A_2 is the solution of

$$4 A_2^2 = \left(\frac{c k_B T_c}{J}\right)^2 - \frac{\sqrt{2} k_B T_c}{\pi J} A_2^{5/2}.$$

Inserting the solution (15) and the assumption (2) in (9), (10) and (11) we find that the critical-point exponents are given by

$$\alpha' = \max\left(0, 1 - x, 1 - \frac{3x}{2}, 2 - \frac{3x}{2}, 2 + x - 2p\right) \tag{16}$$

$$\beta = p - x \tag{17}$$

$$\gamma' = x \tag{18}$$

with x to be taken from (12) and (15).

The examination of α' leads to

$$\alpha' = \begin{cases} 2 - \frac{6p}{5} & 0 < p \leqslant \frac{5}{3} \\ 0 & \frac{5}{3} < p. \end{cases} \tag{19}$$

In the case when $p < 5/3$, the dominant term in the specific heat is

$$c_M = \frac{c^2 k_B^2 T}{2 J A_1}\left[\frac{p^2}{25} + p\,(p - 1)\right] t^{-(2+x-2p)} \tag{20}$$

and because c_M is a positive quantity, we find that p must be greater than 25/26. When $p > 5/3$, c_M tends to $\frac{k_B}{2}$ when $t > 0$.

Using the solution of (12) we can obtain also the critical exponent describing the behaviour of the correlation length. The correlation function for the simple cubic lattice was derived by Berlin and Kac (1952) and it reads

$$G_{s.c.}(r) = < s_j\, s_k > - < s_j > \; < s_k > =$$

$$= \frac{1}{(2\pi)^3\, 4K} \iiint_0^{2\pi} \frac{\cos\left(\frac{\omega_1 x}{a} + \frac{\omega_2 y}{a} + \frac{\omega_3 z}{a}\right) d\omega_1\, d\omega_2\, d\omega_3}{z_s - (\cos\omega_1 + \cos\omega_2 + \cos\omega_3)}$$

which asymptotically, as $r \to \infty$, behaves as (Joyce, 1972)

$$G(r) \approx D_0 \frac{T}{T_c} \frac{a}{r} (1 + k_1 r)\, e^{-k_1 r}$$

where k_1 is the inverse correlation length

$$k_1 = \sqrt{6}\;\sqrt{z_s - 3}$$

Thus the critical exponent ν' is equal to $x/2$ and finally we can make the following table of the critical indices

Table I

p	α'	β	γ'	ν'
$\frac{25}{26} < p \leqslant \frac{5}{3}$	$2 - \frac{6p}{5}$	$\frac{p}{5}$	$\frac{4p}{5}$	$\frac{2p}{5}$
$\frac{5}{3} < p < \frac{5}{2}$	0	$\frac{p}{5}$	$\frac{4p}{5}$	$\frac{2p}{5}$
$\frac{5}{2} \leqslant p$	0	$\frac{1}{2}$	$p - \frac{1}{2}$	$\frac{p}{2} - \frac{1}{4}$

For completeness we quote the remaining critical exponents (Stanley, 1971)

$$\alpha = 0;\ \gamma = 2;\ \Delta = \frac{5}{2};\ \delta = 5;\ \eta = 0;\ \nu = 1.$$

We can easily check that the critical-point indices as given by the first row of table I satisfy a set of relations which are given below

$$
\begin{aligned}
&\alpha' + 2\beta + \gamma' = 2 \\
&\alpha' + \beta(\delta + 1) = 2 \\
&\gamma'(\delta + 1) = (2 - \alpha')(\delta - 1) \\
&\gamma' = \beta(\delta - 1) \\
&d\frac{\delta - 1}{\delta + 1} = 2 - \eta, \quad d = 3 \\
&\frac{d\gamma'}{2 - \alpha'} = \frac{d\gamma'}{2\beta + \gamma'} = 2 - \eta, \quad d = 3 \\
&(2 - \eta)\,\nu' = \gamma' \\
&d\nu' = 2 - \alpha', \qquad d = 3 \\
&\delta = \frac{2 - \alpha' + \gamma'}{2 - \alpha' - \gamma'}
\end{aligned}
\tag{23}
$$

However, at the same time $\gamma \neq \gamma'$. If $p > 5/3$ not all the relations (21) are satisfied. Hence, we conclude that, the temperature-dependent coupling in the spherical Ising model leads to critical-point exponents which automatically satisfy some of the relations which follow from the scaling hypothesis or other assumptions.

A symmetrical to ε' term which is nonzero above the critical temperature will give rise to critical exponents for α and γ which satisfy $\alpha = \alpha'$ and $\gamma = \gamma'$, but at the same time would give nonvanishing magnetization above T_c.

It is interesting to note that for $p = 25/16$ from table I one obtains

$$\alpha' = \frac{1}{8}\,;\ \beta = \frac{5}{16}\,;\ \gamma' = \frac{5}{4}\,;\ \nu' = \frac{5}{8}$$

which are the best, estimated values from seris expansions for the critical-point exponents of the three-dimensional Ising model (Domb, 1974). When $= 5/3$ one gets

$$\alpha' = 0; \quad \beta = \frac{1}{3}; \quad \gamma' = \frac{4}{3}; \quad \nu' = \frac{2}{3}$$

and the exponent $\beta = 1/3$ allows to make the same fit to the experiments as reported by Krizan (1973).

For further work one can attempt to analyze the critical behaviour of an antiferromagnet (Mazo, 1963) or the surface effects (Watson, 1972) when a temperature-dependent coupling is assumed. Above all it would be desirable to find a mechanism for such an interaction.

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ABSTRACT

In the spherical Ising model a temperature-dependent term of the form $-\varepsilon' \sum_i s_i$ is introduced, where $\varepsilon' = ck_B T_c (1 - T/T_c)^p$ when $T \leqslant T_c$ and $\varepsilon' = 0$ when $T > T_c$, while p is a parameter. The critical-point exponents α', β, γ' and ν' are calculated exactly using the solution of Berlin and Kac (1952). It is found that when $25/26 < p \leqslant 5/3$, from the expressions for the critical exponents follow many of the relations which are otherwise derived from the scaling hypothesis.