Multicriticality in the Blume-Capel Model under a Random-Crystal Field Centro Brasileiro de Pesquisas Físicas Facultad de Ciencias Físicas UNMSM

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Blume-Capel Model

$$\mathcal{H} = -\frac{J}{N} \sum_{(i,j)} S_i S_j + \Delta \sum_i S_i^2 \ , \tag{1}$$

where $S_i = -1, 0, 1$, and N is the number of spins.

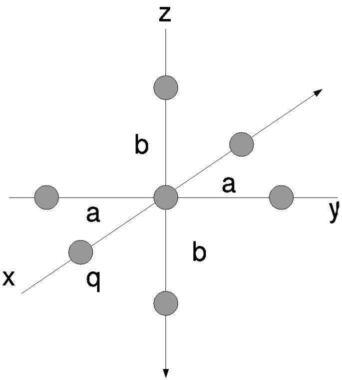


Figure:

An electron at r in an atom at the origin feels an electric potential given by:

$$V(r) = q(\frac{1}{|r - a\hat{x}|} + \frac{1}{|r + a\hat{x}|} + \frac{1}{|r - a\hat{y}|} + \frac{1}{|r + a\hat{y}|} + \frac{1}{|r - b\hat{z}|} + \frac{1}{|r + b\hat{z}|}) \quad (2)$$

By means of the approach

$$\frac{1}{|r \pm a\hat{x}|} \approx \frac{1}{a} \mp \frac{x}{a^2} - \frac{r^2}{2a^3} + \frac{3x^2}{2a^3} \quad (3)$$

valid for $r << a, b$, we obtain

$$V(x, y, z) = q(\frac{1}{b^3} - \frac{1}{a^3})(3z^2 - r^2) + constant \quad (4)$$

In order to describe a magnetic ion in the crystal we have to add the magnetic interaction to the contribution of the crystal field, so

$$H = -B_0 S_z + A(3z^2 - r^2) \tag{5}$$

By means of the Wigner-Eckart Theorem:

$$H_{crystal} \; \alpha \; (3S_z^2 - S^2) \tag{6}$$

,

Close to a continuous-phase transition,

$$m = A_1 m + A_3 m^3 + A_5 m^5 + A_7 m^7 \dots \tag{7}$$

Continuous frontier:

$$A_1 = 1,\ A_3 < 0,\ A_5 < 0\ , \tag{8}$$

Tricritical point:

$$A_1 = 1,\ A_3 = 0,\ A_5 < 0\ . \tag{9}$$

Fourth order point:

$$A_1 = 1,\ A_3 = 0,\ A_5 = 0\ A_7 < 0\ . \tag{10}$$

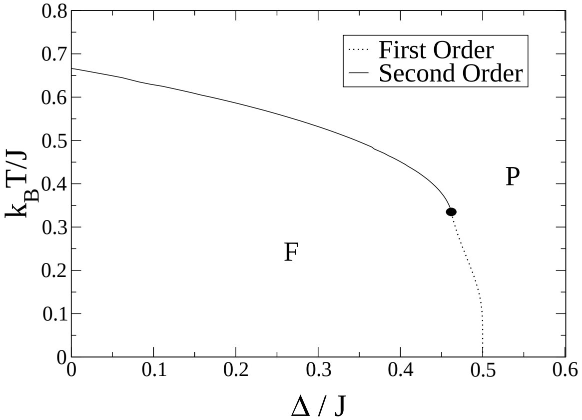


Figure: Phase diagram of the Blume-Capel model in the plane $k_B T/J - \Delta/J$ within the mean-field approach

$$\mathcal{H} = -\frac{J}{N}\sum_{(i,j)}\sigma_i\sigma_j + \sum_i h_i\sigma_i \tag{11}$$

$\sigma = \pm 1$

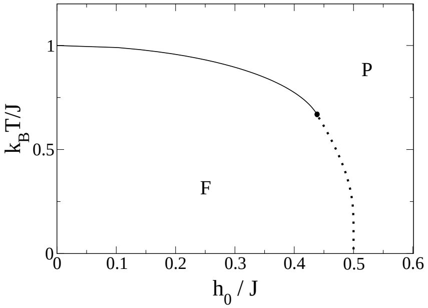
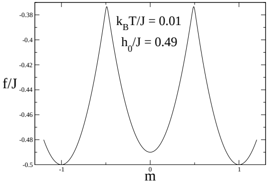
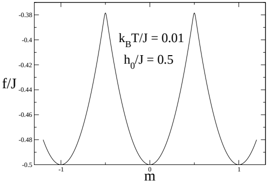


Figure: Random-Field Ising Model (RFIM) in the mean-field approach.


k_BT/J = 0.01
h_0/J = 0.49
f/J
m
-0.38
-0.4
-0.42
-0.44
-0.46
-0.48
-0.5
-1
0
1

(a)


k_BT/J = 0.01
h_0/J = 0.5
f/J
m
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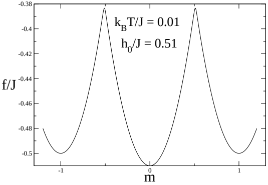
-0.4
-0.42
-0.44
-0.46
-0.48
-0.5
-1
0
1

(b)


k_BT/J = 0.01
h_0/J = 0.51
f/J
m
-0.38
-0.4
-0.42
-0.44
-0.46
-0.48
-0.5
-1
0
1

(c)

$$\mathcal{H} = -\frac{J}{N} \sum_{(i,j)} S_i S_j + \sum_i \Delta_i S_i^2 \ , \qquad (12)$$

where $S_i = -1, 0, 1$, and N is the number of spins. The sum runs over all pairs of spins. The Crystal Field (a quenched variable) obeys:

$$P(\Delta_i) = \frac{p}{\sqrt{2\pi}\,\sigma} \exp\left[-\frac{(\Delta_i - \Delta)^2}{2\sigma^2}\right] + \frac{(1-p)}{\sqrt{2\pi}\,\sigma} \exp\left[-\frac{{\Delta_i}^2}{2\sigma^2}\right] \ , \qquad (13)$$

$$f = \frac{1}{2} J m^2 - \frac{1}{\beta} E \left\{ \log(2 \exp(-\beta \Delta_i) \cosh(\beta J m) + 1) \right\} \ , \qquad (14)$$

$$m = \sinh(\beta m) E \left\{ \left[\cosh(\beta m) + \frac{1}{2} \exp(\beta \Delta_i) \right]^{-1} \right\} \ , \qquad (15)$$

where the quenched average, represented by $E\{...\}$, is taken with respect to the PDF, and $\beta = 1/(k_B T)$

$$m = A_1 m + A_3 m^3 + A_5 m^5 + A_7 m^7 + \ldots , \tag{16}$$

where

$$A_1 = \beta E\{g_i\} , \tag{17}$$

$$A_3 = \beta^3 E\{(\frac{1}{6} g_i - \frac{1}{2} g_i^2)\} , \tag{18}$$

$$A_5 = \beta^5 E\{(\frac{1}{120} g_i - \frac{1}{8} g_i^2 + \frac{1}{4} g_i^3)\} , \tag{19}$$

$$A_7 = \beta^7 E\{(\frac{1}{5040} g_i - \frac{1}{80} g_i^2 + \frac{1}{12} g_i^3 - \frac{1}{8} g_i^4)\} , \tag{20}$$

and

$$g_i = (1 + \frac{1}{2} \exp(\beta \Delta_i))^{-1} . \tag{21}$$

By taking $\beta \to \infty$ ($T \to 0$), we get the asymptotic limit of the free energy and the magnetization, so we have

$$\begin{aligned} f &= \frac{1}{2}Jm^2 - p(\frac{1}{2}(Jm-\Delta)\left(1+\mathrm{erf}\left[\frac{Jm-\Delta}{\sqrt{2}\,\sigma}\right]\right) \\ &+ \frac{\sigma}{\sqrt{2\pi}}\exp\left[-\frac{(Jm-\Delta)^2}{2\,\sigma^2}\right]) \\ &- (1-p)\left(\frac{1}{2}Jm\left(1+\mathrm{erf}\left[\frac{Jm}{\sqrt{2}\,\sigma}\right]\right)+\frac{\sigma}{\sqrt{2\pi}}\exp\left[-\frac{J^2m^2}{2\,\sigma^2}\right]\right) \end{aligned} \quad (22)$$

$$m = \frac{p}{2}\left(1+\mathrm{erf}\left[\frac{Jm-\Delta}{\sqrt{2}\,\sigma}\right]\right)+\frac{(1-p)}{2}\left(1+\mathrm{erf}\left[\frac{Jm}{\sqrt{2}\,\sigma}\right]\right)\ , \quad (23)$$

where

$$\mathrm{erf}\left(\frac{x}{\sqrt{2}}\right) = \sqrt{\frac{2}{\pi}}\int_0^x dz e^{-z^2/2}\ . \quad (24)$$

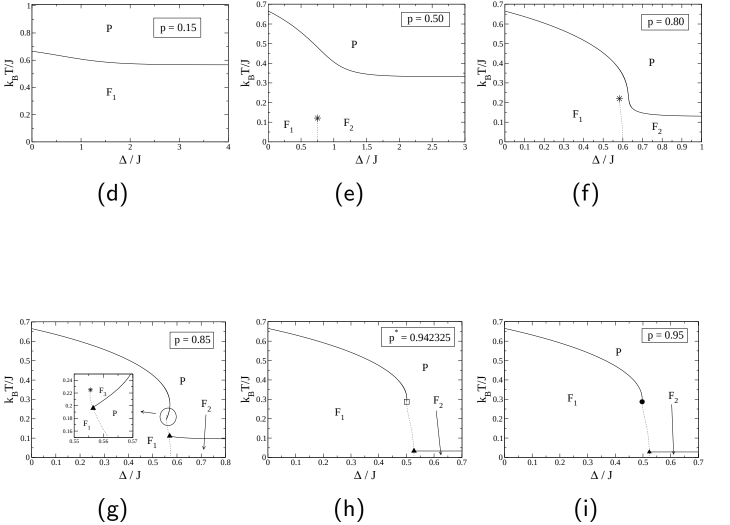


Figure: For $\sigma/J = 0.1$, the diagrams show a variety of topologies according to the probability p.

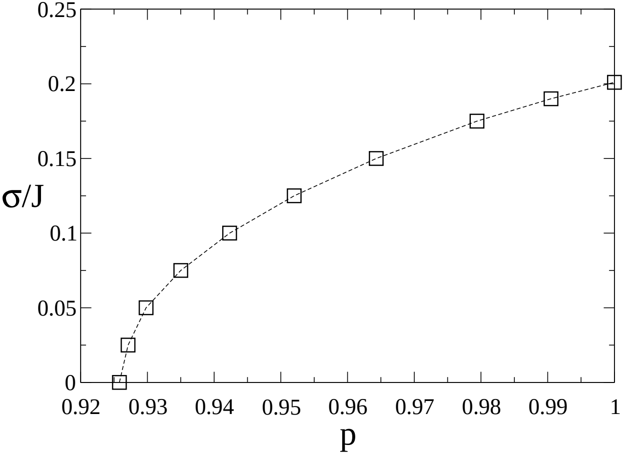
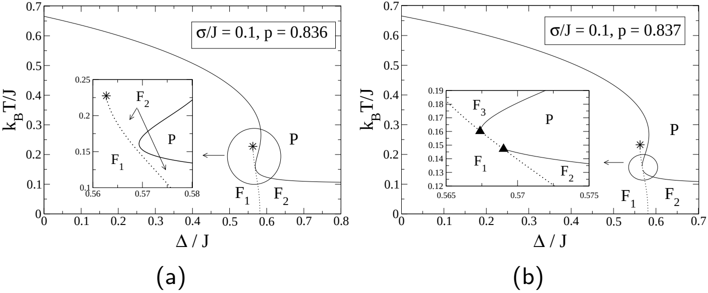


Figure: Some fourth-order critical points located in the plane $p - \sigma/J$.



(a) (b)

Figure: Phase diagrams (for $\sigma/J = 0.1$) showing two slightly different values of p, between which there is a critical p for passing from Topology II to III. So, that critical point must be found for $p = 0.8365 \pm 0.0005$.

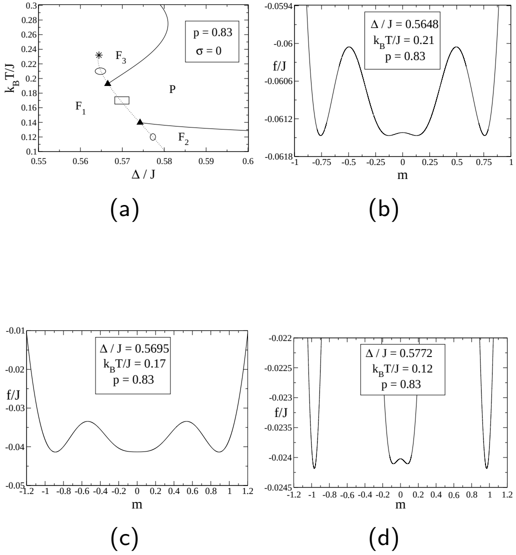
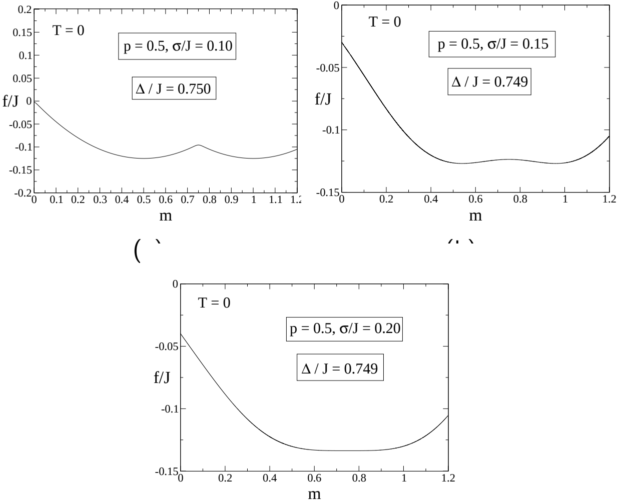
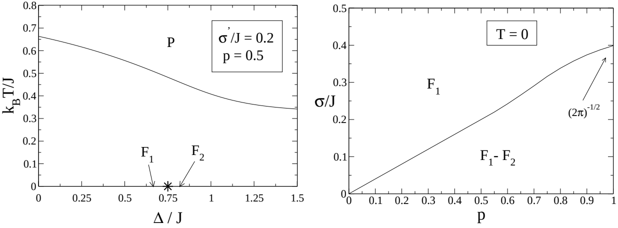


Figure: In (a) is shown the most critical region of the phase diagram for $\sigma = 0$, and $p = 0.83$.


T = 0
p = 0.5, σ/J = 0.10
Δ / J = 0.750
f/J
m
T = 0
p = 0.5, σ/J = 0.15
Δ / J = 0.749
f/J
m
T = 0
p = 0.5, σ/J = 0.20
Δ / J = 0.749
f/J
m

(c)

Figure:



(a) (b)

Figure: In (a) is shown the phase diagram obtained for $p = 0.5$, for the corresponding critical σ'/J. Note that the ordered-critical point (that appeared in Topology II) is now located at the horizontal axis. So, for $\sigma > \sigma'$ there will be only one ferromagnetic order at low temperatures for $p = 0.5$. In (b), the line separating topologies I and II. This line is made of points numerically obtained by finding σ'/J, for each p.

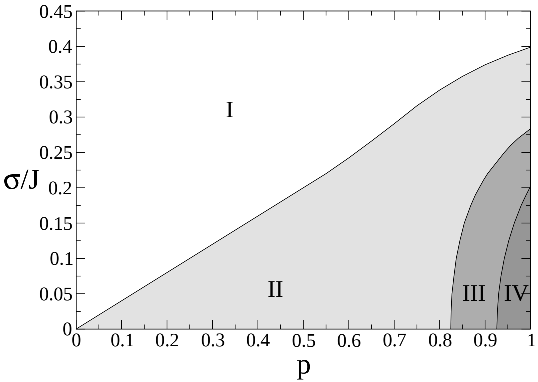


Figure: Regions, in the plane σ/J versus p, associated with the topologies for the present model (see also Figure 2). The horizontal and the vertical axes represent the probability p, and the width σ, respectively (see Eq. (**??**)). The tricritical behavior belongs to the region IV. The simplest topology belongs to region I, where only one ferromagnetic phase appears, whereas the rest topologies contain two ferromagnetic orders at low temperatures.