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LETTER TO THE EDITOR

The tri-critical point in the Blume–Emery–Griffiths model

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Abstract. The tri-critical behaviour of the spin-one Blume–Emery–Griffiths Ising model is investigated by means of the recently developed effective-field theory based on an extension of the Honmura–Kaneyoshi technique. The dependence of the position of the tri-critical point on the relative strengths of the bi-quadratic and bi-linear exchange interactions is investigated for the honeycomb, square and cubic lattices.

Recently, we considered the application of the effective-field theory (EFT) based on the differential operator technique of Honmura and Kaneyoshi (1979) to the Blume–Emery–Griffiths (BEG) model (Tucker 1988). We pointed out that a previous version of the theory presented by Fittipaldi and Siqueira (1986) contains an unfortunate error that leads to results that are in some cases even qualitatively wrong. A correct treatment of the effective field equations was presented and it was found that the results then obtained resembled those of the cluster variational method in pair approximation, and of other methods. In that paper we considered only the isotropic BEG model in which the single-ion anisotropy is absent. The anisotropic model is, however, more interesting, in that for certain values of the single-ion anisotropy the system possesses a tri-critical point at which the phase transition changes from second to first order. The usefulness of EFT in studying tri-critical points was demonstrated by Kaneyoshi (1986, 1987a) in the case of the Blume–Capel model (the BEG model with zero bi-quadratic exchange). However, recent applications of the method of the BEG model (Kaneyoshi 1987b, Kaneyoshi *et al* 1988, Kaneyoshi and Sarmento 1988) are defective in that they use as their starting point the effective-field equations of Fittipaldi and Siqueira referred to above. The purpose of this Letter is to study the tri-critical points using our version of the effective-field theory. General expressions that enable the tri-critical points in the BEG model to be obtained are derived and numerical values for the honeycomb, square and cubic lattices presented.

The Hamiltonian of the spin-1 BEG model is given by

$$H = -J\sum_{\langle ij\rangle} S_{iz}S_{jz} - J'\sum_{\langle ij\rangle} S_{iz}^2 S_{jz}^2 + D\sum_i S_{iz}^2 \tag{1}$$

where J and J' are the nearest-neighbour bi-linear and bi-quadratic exchange constants and D is the single-ion anisotropy. In discussing the results it is conventional to introduce the notation $\alpha = J'/J$ and $\alpha' = D/Jz$ where z is the coordination number of the lattice. As shown by Siqueira and Fittipaldi (1985), use of an extended Honmura–Kaneyoshi technique enables the expressions for the magnetisation and the quadrupolar moment to be cast in the form

$$m = \langle S_{gz} \rangle = \langle \exp(D_x \beta E_d + D_y \beta E_q) \rangle f(x, y)|_{x\to 0, y\to 0} \tag{2}$$

$$q = \langle S_{gz}^2 \rangle = \langle \exp(D_x \beta E_d + D_y \beta E_q) \rangle g(x, y)|_{x\to 0, y\to 0} \tag{3}$$

with

$$E_d = J \sum_{\delta} S_{\delta z} \qquad E_q = \alpha J \sum_{\delta} S_{\delta z}^2 - D \qquad D_x \equiv \partial/\partial x \qquad D_y \equiv \partial/\partial y$$

and

$$f(x, y) = 2\exp(y)\sinh(x)/(1 + 2\exp(y)\cosh(x))$$

$$g(x, y) = 2\exp(y)\cosh(x)/(1 + 2\exp(y)\cosh(x)).$$

The summation over δ is over the nearest neighbour of g. Using the Van der Waerden identities for the spin-1 Ising system and neglecting correlations between different spins, one can then show that

$$m = [P(D_x, D_y; m, q)]^z f(x, y - \beta D)|_{x=0, y=0} \tag{4}$$

$$q = [P(D_x, D_y; m, q)]^z g(x, y - \beta D)|_{x=0, y=0} \tag{5}$$

with

$$P(D_x, D_y; m, q) = 1 + m\sinh(\beta J D_x)\exp(\beta\alpha J D_y) + q(\exp(\beta\alpha J D_y)\cosh(\beta J D_x) - 1). \tag{6}$$

Equations (4) and (5) extend (10) and (11) of our earlier work (Tucker 1988) to the anisotropic case. In order to study the second-order phase transitions and the tri-critical points we follow the work of Kaneyoshi (1986) and expand the right-hand side of (4) and (5) as power polynomials in m. That is

$$m = A(q)m + B(q)m^3 + C(q)m^5 \tag{7}$$

$$q = A'(q) + B'(q)m^2 + C'(q)m^4 \tag{8}$$

where the coefficients $A(q)$, $B(q)$ etc are dependent on q in addition to temperature and the parameters α and α'. In particular we find

$$A(q) = \sum_{r=1}^{z} a_r^z \sum_{p=0}^{<r/2} \frac{(r-1)!(r-2p)}{p!(r-p)!} F_{r,r-2p} \tag{9}$$

$$A'(q) = \sum_{r=0}^{z} b_r^z \sum_{p=0}^{\leq r/2} \frac{r!}{p!(r-p)!} G_{r,r-2p} \tag{10}$$

$$B(q) = \sum_{r=3}^{z} e_r^z \left(\sum_{p=0}^{<r/2} \frac{(r-1)!(r-2p)}{p!(r-p)!} F_{r,r-2p} - 4 \sum_{p=0}^{<(r-2)/2} \frac{(r-3)!(r-2-2p)}{p!(r-2-p)!} F_{r,r-2-2p} \right) \tag{11}$$

$$B'(q) = \sum_{r=2}^{z} f_r^z \left(\sum_{p=0}^{\leq r/2} \frac{r!}{p!(r-p)!} G_{r,r-2p} - 4 \sum_{p=0}^{\leq (r-2)/2} \frac{(r-2)!}{p!(r-2-p)!} G_{r,r-2-2p} \right) \tag{12}$$

$$C(q)=\sum_{r=5}^{z} g_r^z\left(\sum_{p=0}^{<r/2}\frac{(r-1)!(r-2p)}{p!(r-p)!}F_{r,r-2p}\right.$$
$$-8\sum_{p=0}^{<(r-2)/2}\frac{(r-3)!(r-2-2p)}{p!(r-2-p)!}F_{r,r-2-2p}$$
$$\left.+16\sum_{p=0}^{<(r-4)/2}\frac{(r-5)!(r-4-2p)}{p!(r-4-p)!}F_{r,r-4-2p}\right) \tag{13}$$

$$C'(q)=\sum_{r=4}^{z} h_r^z\left(\sum_{p=0}^{\leqslant r/2}\frac{r!}{p!(r-p)!}G_{r,r-2p}-8\sum_{p=0}^{\leqslant(r-2)/2}\frac{(r-2)!}{p!(r-2-p)!}G_{r,r-2-2p}\right.$$
$$\left.+16\sum_{p=0}^{\leqslant(r-4)/2}\frac{(r-4)!}{p!(r-4-p)!}G_{r,r-4-2p}\right) \tag{14}$$

where

$$a_r^z=\frac{z!(1-q)^{z-r}q^{r-1}}{2^r(r-1)!(z-r)!} \qquad b_r^z=\frac{z!(1-q)^{z-r}q^r}{2^r r!(z-r)!}$$
$$e_r^z=\frac{z!(1-q)^{z-r}q^{r-3}}{3!2^r(r-3)!(z-r)!} \qquad f_r^z=\frac{z!(1-q)^{z-r}q^{r-2}}{2!2^r(r-2)!(z-r)!} \tag{15}$$
$$g_r^z=\frac{z!(1-q)^{z-r}q^{r-5}}{5!2^r(r-5)!(z-r)!} \qquad h_r^z=\frac{z!(1-q)^{z-r}q^{r-4}}{4!2^r(r-4)!(z-r)!}$$

and

$$F_{rp}=\frac{4\exp(r\beta\alpha J)\sinh(p\beta J)}{\exp(\beta Jz\alpha')+2\exp(r\beta\alpha J)\cosh(p\beta J)} \tag{16}$$

$$G_{rp}=\frac{4\exp(r\beta\alpha J)\cos(p\beta J)}{\exp(\beta Jz\alpha')+2\exp(r\beta\alpha J)\cosh(p\beta J)}(1-\tfrac{1}{2}\delta_{p,0}). \tag{17}$$

Note that because we restricted the index p to positive values, the quantities F_{rp} and G_{rp} ($p\neq 0$) have been defined with an extra factor of 2 compared to $f(x,y)$ and $g(x,y)$. Most frequently, one is interested in lattices with coordination number $z\leqslant 6$, in which case (9) to (14) reduce to

$$A(q)=a_1^zF_{11}+a_2^zF_{22}+a_3^z(F_{33}+F_{31})+a_4^z(F_{44}+2F_{42})+a_5^z(F_{55}+3F_{53}+2F_{51})$$
$$+a_6^z(F_{66}+4F_{64}+5F_{62}) \tag{18}$$

$$A'(q)=b_0^zG_{00}+b_1^zG_{11}+b_2^z(G_{22}+2G_{20})+b_3^z(G_{33}+3G_{31})+b_4^z(G_{44}+4G_{42}+6G_{40})$$
$$+b_5^z(G_{55}+5G_{53}+10G_{51})+b_6^z(G_{66}+6G_{64}+15G_{62}+20G_{60}) \tag{19}$$

$$B(q)=e_3^z(F_{33}-3F_{31})+e_4^z(F_{44}-2F_{42})+e_5^z(F_{55}-F_{53}-2F_{51})$$
$$+e_6^z(F_{66}-3F_{62}) \tag{20}$$

$$B'(q)=f_2^z(G_{22}-2G_{20})+f_3^z(G_{33}-G_{31})+f_4^z(G_{44}-2G_{40})$$
$$+f_5^z(G_{55}+G_{53}-2G_{51})+f_6^z(G_{66}+2G_{64}-G_{62}-4G_{60}) \tag{21}$$

$$C(q)=g_5^z(F_{55}-5F_{53}+10F_{51})+g_6^z(F_{66}-4F_{64}+5F_{62}) \tag{22}$$

$$C'(q) = h_4^z(G_{44} - 4G_{42} + 6G_{40}) + h_5^z(G_{55} - 3G_{53} + 2G_{51}) + h_6^z(G_{66} - 2G_{64} - G_{62} + 4G_{60}). \tag{23}$$

At this stage one can make contact with the work of Siqueira and Fittipaldi (1986) on the Blume–Capel model. For that model F_{rp} and G_{rp} are independent of the subscript r and the coefficients $A(q)$, $A'(q)$, $B(q)$, $B'(q)$, $C(q)$ and $C'(q)$ should reduce to their coefficients $A_{1z} + 1$, $B_{0z} + q$, A_{3z}, B_{2z}, A_{5z} and B_{4z}, respectively, tabulated in the appendix of that reference. Agreement is obtained except in the following cases. We find

$$A_{13} = 3R^2 f(K) + 3Rqf(2K) + \tfrac{3}{4}q^2(f(3K) + f(K)) - 1$$

$$A_{33} = \tfrac{1}{4}(f(3K) - 3f(K))$$

$$A_{34} = R(f(3K) - 3f(K)) + \tfrac{1}{2}q(f(4K) - 2f(K))$$

$$B_{24} = 3R^2(g(2K) - g_0) + 3Rq(g(3K) - g(K)) + \tfrac{3}{4}q^2(g(4K) - g_0)$$

and the fourth term in A_{16} should contain the factor R^2 rather than R. (There are also trivial misprints in that $gg(K)$ should be $qg(K)$ everywhere and a superfluous r appears in A_{14}).

In the neighbourhood of a second-order transition line where m is small one may write for the state equations

$$m = am + bm^3 + cm^5 + \dots \tag{24}$$

$$q = q_0 + q_1 m^2 + q_2 m^4 + \dots . \tag{25}$$

It follows, on substituting the expression for q into the right-hand side of (8) and performing a Taylor expansion, that q_0 is the solution of

$$q_0 = A'(q_0) \tag{26}$$

and q_1 and q_2 are given by

$$q_1 = B'(q_0) \Big/ \left(1 - \left.\frac{\partial A'}{\partial q}\right|_{q_0}\right) \tag{27}$$

$$q_2 = \left(\frac{1}{2}\left.\frac{\partial^2 A'}{\partial q^2}\right|_{q_0} q_1^2 + \left.\frac{\partial B'}{\partial q}\right|_{q_0} q_1 + C'(q_0)\right) \Big/ \left(1 - \left.\frac{\partial A'}{\partial q}\right|_{q_0}\right). \tag{28}$$

Likewise from (7) and (24) one finds that

$$a = A(q_0) \tag{29}$$

$$b = \left.\frac{\partial A}{\partial q}\right|_{q_0} q_1 + B(q_0) \tag{30}$$

$$c = \left.\frac{\partial A}{\partial q}\right|_{q_0} q_2 + \frac{1}{2}\left.\frac{\partial^2 A}{\partial q^2}\right|_{q_0} q_1^2 + \left.\frac{\partial B}{\partial q}\right|_{q_0} q_1 + C(q_0). \tag{31}$$

As pointed out for example by Benayad *et al* (1985), the second-order transition line is given by $a = 1$ and $b < 0$, and a tri-critical point ocurs at $a = 1$, $b = 0$ if $c < 0$. Using these criteria we have located the position of the tri-critical points for the honeycomb, square and cubic lattices for several values of α. The coordinates of the tricritical point in the

Table 1. Coordinates of the tri-critical points in the (α', $1/\beta J$) plane.

	$z=3$		$z=4$		$z=6$	
α	α'	$1/\beta J$	α'	$1/\beta J$	α'	$1/\beta J$
0.0	0.475	0.68	0.472	1.01	0.468	1.67
0.1	0.519	0.74	0.513	1.11	0.506	1.85
0.2	0.563	0.81	0.554	1.21	0.543	2.01
0.3	0.606	0.87	0.594	1.30	0.580	2.17
0.4	0.648	0.93	0.634	1.39	0.617	2.31
0.5	0.690	0.99	0.674	1.47	0.654	2.45

(α', $1/\beta J$) plane are tabulated in table 1 for these lattices. In the absence of bi-quadratic exchange ($\alpha = 0$) the values may be compared to those obtained by other methods for the Blume–Capel model which are quoted in Siqueira and Fittipaldi (1986). In this Letter we have only presented numerical results for a range of bi-quadratic exchange strengths where the critical frontier for the second-order transition is relatively well behaved. However, it is hoped that the general expressions presented here will prove useful in a thorough investigation of the phase diagram, particularly in the regime where $J + J' < 0$, where it has been conjectured that a new type of disordered phase might exist (Kaneyoshi 1987b).

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