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Critical properties of the Ashkin–Teller model from the mean-field renormalisation group approach†

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Abstract. By using small size clusters, which carry all the basic symmetries of the Ashkin-Teller model, we obtain within the mean-field renormalisation group approach the complete phase diagram of the model. Estimates of the thermal critical exponent are also obtained.

The Ashkin-Teller model (ATM) is a generalisation of the Ising model to a four-component system. In this case, each site of the lattice is occupied by one of four different types of atoms A, B, C or D (Ashkin and Teller 1943). In terms of spin variables it can be considered as two superposed spin-$\frac{1}{2}$ Ising models described, respectively, by σ_i and S_i sitting on each of the sites of a d-dimensional hypercubic lattice (Fan 1972). Within each Ising model there is a two-spin nearest-neighbour interaction J_2 and the different Ising models are coupled by a four-spin interaction J_4. The Hamiltonian can then be written as

$$-\beta\mathscr{H} = H = \sum_{\langle ij\rangle} [K_2(\sigma_i\sigma_j + S_iS_j) + K_4\sigma_i\sigma_jS_iS_j] \tag{1}$$

where $\beta = (k_B T)^{-1}$, $K_2 = \beta J_2$ and $K_4 = \beta J_4$. This model has a very rich phase diagram. Although some exact results are known for the two-dimensional model (Fan and Wu 1970, Knops 1975, Baxter 1982 and references therein) only mean-field results are available for $d > 2$ (Ditzian *et al* 1980, Cristiano and Goulart Rosa 1984).

In this paper we study the critical properties of the ATM through the mean-field renormalisation group (MFRG) approach (Indekeu *et al* 1982). We consider herein just the simplest choice for the clusters, namely one- and two-site clusters.

The Hamiltonian for the one-site cluster is

$$H_1 = ZK_2'\sigma_1 h_\sigma' + ZK_2'S_1 h_S' + ZK_4'\sigma_1 S_1 h_{\sigma S}' \tag{2}$$

where Z is the lattice coordination number and h_σ', h_S' and $h_{\sigma S}'$ are the symmetry breaking boundary fields simulating the effect of the infinite system. The order parameters associated with the spin variables σ, S and σS obtained from the Hamiltonian

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(2) are easily evaluated:

$$m'_\sigma = \langle\sigma\rangle_1 = (t'_\sigma + t'_S t'_{\sigma S})/D' \tag{3a}$$

$$m'_S = \langle S\rangle_1 = (t'_S + t'_\sigma t'_{\sigma S})/D' \tag{3b}$$

$$m'_{\sigma S} = \langle\sigma S\rangle_1 = (t'_{\sigma S} + t'_\sigma t'_S)/D' \tag{3c}$$

$$D' = 1 + t'_\sigma t'_S t'_{\sigma S} \tag{3d}$$

where

$$t'_\sigma = \tanh ZK'_2 h'_\sigma \qquad t'_S = \tanh ZK'_2 h'_S \qquad t'_{\sigma S} = \tanh ZK'_4 h'_{\sigma S}. \tag{3e}$$

Relations (3) are just the mean-field equations when the symmetry breaking fields are approximated by their order parameters (Ditzian *et al* 1980).

The Hamiltonian for the two-site cluster reads

$$H_2 = K_2(\sigma_1\sigma_2 + S_1S_2) + K_4\sigma_1S_1\sigma_2S_2 + (Z-1) \times [K_2(\sigma_1+\sigma_2)h_\sigma + K_2(S_1+S_2)h_S + K_4(\sigma_1S_1+\sigma_2S_2)h_{\sigma S}]. \tag{4}$$

Similarly, we obtain

$$m_\sigma = \langle\sigma\rangle_2 = (t_\sigma + t_S t_{\sigma S} + Xt_\sigma/c_S c_{\sigma S})/D \tag{5a}$$

$$m_S = \langle S\rangle_2 (t_S + t_\sigma t_{\sigma S} + Xt_S/c_\sigma c_{\sigma S})/D \tag{5b}$$

$$m_{\sigma S} = \langle\sigma S\rangle_S = (t_{\sigma S} + t_\sigma t_S + Yt_{\sigma S}/c_\sigma c_S)/D \tag{5c}$$

$$D = 1 + t_\sigma t_S t_{\sigma S} + X/c_S c_{\sigma S} + X/c_\sigma c_{\sigma S} + Y/c_\sigma c_S \tag{5d}$$

where

$$t_\sigma = \tanh 2(Z-1)K_2h_\sigma \qquad t_S = \tanh 2(Z-1)K_2h_S \qquad t_{\sigma S} = \tanh 2(Z-1)K_4h_{\sigma S}$$

$$c_\sigma = \cosh 2(Z-1)K_2h_\sigma \qquad c_S = \cosh 2(Z-1)K_2h_S \qquad c_{\sigma S} = \cosh 2(Z-1)K_4h_{\sigma S} \tag{5e}$$

$$X = \exp(-2K_2 - 2K_4) \qquad Y = \exp(-4K_2).$$

The critical properties of the ATM are obtained by assuming that the approximated magnetisations scale as $m'_i = \xi_i m_i$ ($i = \sigma$, S or σS) and imposing a similar relation for the symmetry breaking fields, i.e. $h'_i = \xi_i h_i$ (Indekeu *et al* 1982). As in $d = 2$ all the phase transition lines of the ATM are of second order, the respective symmetry breaking field must be considered very small. The equations obtained from the scaling relation between these two clusters are then independent of ξ_i and can be viewed as a renormalisation recursion relation among the Hamiltonian parameters (K'_2, K'_4) and (K_2, K_4). Due to the fact that this model contains two different interaction couplings, the complete flow diagram in the parameter space cannot be obtained. However, estimates of the critical exponent ν, associated with some invariant sets in the (K_2, K_4) space, can be calculated through $(\partial K'_2/\partial K_2)_{FP} = l^{1/\nu}$, where $l = 2^{1/d}$ and the derivative is taken at the fixed point of the particular invariant set considered.

Although the present formalism, as can be seen from equations (3) and (5), can easily be extended to any dimension, in what follows we will be mainly concerned with the two-dimensional model, where several exact results are available.

Figure 1 shows the phase diagram of the ATM in $d = 2$. In the phase labelled as 'Baxter' we have $\langle\sigma\rangle \neq 0$, $\langle S\rangle \neq 0$ and $\langle\sigma S\rangle \neq 0$ while in the paramagnetic phase ('para') neither σ nor S (nor the product σS) are ordered. In the '$\langle\sigma S\rangle$' phase we have σ and S disordered ($\langle\sigma\rangle = 0$ and $\langle S\rangle = 0$) with $\langle\sigma S\rangle$ ordered ferromagnetically. The '$\langle\sigma S\rangle_{AF}$' phase is similar to the '$\langle\sigma S\rangle$' phase but in this case $\langle\sigma S\rangle$ is ordered antiferromagnetically.

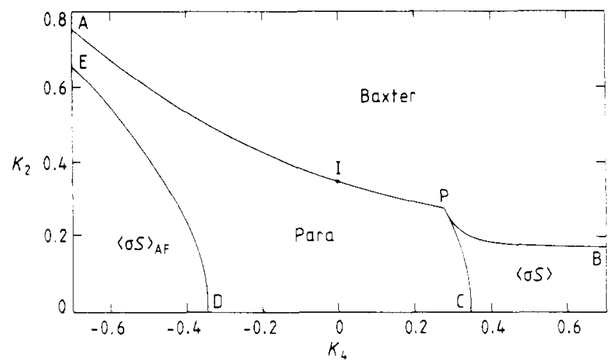

Figure 1. Phase diagram of the Ashkin–Teller model in two dimensions obtained from the present approach.

The transition from the 'Baxter' to the 'para' phase is characterised by the vanishing of all order parameters. Thus, for small fields, equations (3) and (5) can be written as

$$m'_\sigma = ZK'_2 h'_\sigma \qquad m'_S = ZK'_2 h'_S \qquad m'_{\sigma S} = ZK'_4 h'_{\sigma S} \tag{6}$$

and

$$\begin{aligned} m_\sigma &= (1+X)2(Z-1)K_2 h_\sigma / D_0 \\ m_S &= (1+X)2(Z-1)K_2 h_S / D_0 \\ m_{\sigma S} &= (1+Y)2(Z-1)K_4 h_{\sigma S} / D_0 \end{aligned} \tag{7}$$

where $D_0 = 1+2X+Y$. From the scaling relation between m'_σ, m'_S and m_σ, m_S we obtain

$$ZK'_2 = [(1+X)2(Z-1)K_2]/D_0 \tag{8}$$

which is interpreted as a renormalisation recursion relation among the Hamiltonian parameters. The fixed point solution of (8), namely

$$K_2 = \tfrac{1}{2}\ln(Z/\{[\exp(-4K_4) + Z(Z-2)]^{1/2} - \exp(-2K_4)\}) \tag{9}$$

gives the phase transition line where both σ and S (and, of course, $\langle\sigma S\rangle$) independently order. Equation (9) corresponds to the AIP line on the phase diagram shown in figure 1.

In the transition from the 'para' to the '$\langle\sigma S\rangle$' phase only $\langle\sigma S\rangle$ orders while σ and S remain disordered. From the scaling relation between $m'_{\sigma S}$ and $m_{\sigma S}$, given in (6) and (7), one has

$$ZK'_4 = (1+Y)2(Z-1)K_4/D_0. \tag{10}$$

The fixed point solution of (10) is

$$K_2 = \tfrac{1}{2}\ln(\{Z\exp(-2K_4)/(Z-2) - [Z^2\exp(-4K_4)/(Z-2)^2 - 1]^{1/2}\}^{-1}) \tag{11}$$

and corresponds to the PC line in figure 1. The transition line from the 'para' to the '$\langle\sigma S\rangle_{AF}$' phase is obtained in a similar way. We have, in this case, to consider $K_4 < 0$ and adjust the field $h_{\sigma S}$ in an antiferromagnetic way. The final result for the fixed point solution so obtained for the ED transition line is

$$K_2 = \tfrac{1}{2}\cosh^{-1}[(Z-2)\exp(2K_4)/Z]. \tag{12}$$

Obtaining the transition from the 'Baxter' to the '$\langle\sigma S\rangle$' phase is more subtle. In this case, σ and S disorder at the transition while $\langle\sigma S\rangle$ remains different from zero.

Therefore, for small fields associated with the variables σ and S equations (3) and (5) read

$$m'_\sigma = ZK'_2h'_\sigma + ZK'_2h'_St'_{\sigma S} \qquad m'_S = ZK'_2h'_S + ZK'_2h'_\sigma t'_{\sigma S} \qquad m'_{\sigma S} = t'_{\sigma S} \tag{13}$$

and

$$\begin{aligned} m_\sigma &= [(1 + X/c_{\sigma S})2(Z-1)K_2h_\sigma + 2(Z-1)K_2h_St_{\sigma S}]/D_1 \\ m_S &= [(1 + X/c_{\sigma S})2(Z-1)K_2h_S + 2(Z-1)K_2h_\sigma t_{\sigma S}]/D_1 \\ m_{\sigma S} &= (1+Y)t_{\sigma S}/D_1 \end{aligned} \tag{14}$$

where

$$D_1 = 1 + Y + 2X/c_{\sigma S}.$$

As can be seen from equations (13) and (14) the order parameters associated with σ and S are now dependent on both scaling fields. On the other hand, in this transition we expect that $\langle\sigma\rangle = \langle S\rangle$. Therefore, taking $m'_\sigma = m'_S$ and $m_\sigma = m_S$ with the same relations for the respective scaling fields one obtains

$$(1 + t'_{\sigma S})zK'_2 = (1 + t_{\sigma S} + X/c_{\sigma S})2(Z-1)K_2/D_1. \tag{15}$$

The above equation still depends on the fields $h'_{\sigma S}$ and $h_{\sigma S}$ reflecting the fact that $\langle\sigma S\rangle \neq 0$. This variable has its own size dependence which is not governed by finite-size scaling along this transition line. It is then reasonable to assume that $m'_{\sigma S} = m_{\sigma S}$ and $h'_{\sigma S} = h_{\sigma S}$ obtaining

$$t'_{\sigma S} = (1+Y)t_{\sigma S}/D_1 \qquad h'_{\sigma S} = h_{\sigma S}. \tag{16}$$

The PB critical line is given by the fixed point solutions of equation (15) where $h_{\sigma S}$ is eliminated via equation (16). The assumption used here to treat the non-critical behaviour associated with the variable σS is conceptually different from the mean-field ansatz used in the treatment of the antiferromagnetic Ising model on the triangular lattice (Slotte 1984) and the spin-1 biquadratic Ising model (Alcantara Bonfim and Sá Barreto 1985). In the present case, we are able to compute an approximate mean value $\langle\sigma S\rangle$ as a function of the temperature along the PB line as shown in figure 2. It is clear from this figure that the physically expected behaviour for this variable is obtained.

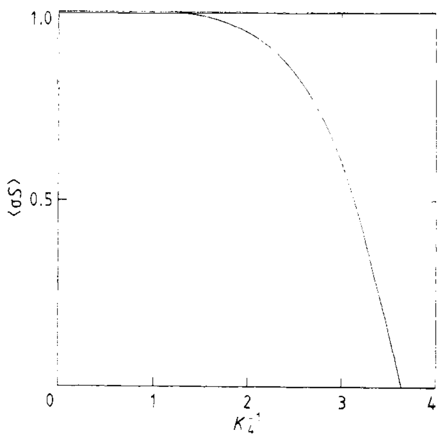

Figure 2. Mean value $\langle\sigma S\rangle$ as a function of K_4 along the transition line from the 'Baxter' to the '$\langle\sigma S\rangle$' phase. K_2 is not shown.

In contrast, within the mean-field ansatz, the thermal behaviour of the non-critical variable is not uniquely defined (once it has different values for the different clusters) and the point P is no more a bifurcation point.

At the decoupling point, $K_4=0$, $K_I=0.346$ which should be compared with the exact value $K_I=0.441$. The point P, as shown by exact arguments, corresponds to the four-state Potts model and is located at $K_2=K_4$. In the present approach we have $K_2=K_4=K_P=0.275$, a value that has been previously obtained by Indekeu *et al* (1982) studying the q-state Potts model by using the same size clusters and for $q=4$. The following exact relations are also obtained: $K_B=K_I/2$ and $K_C=K_I=-K_D$. Moreover, for $K_2=-K_4$ equation (9) gives

$$K_2=-K_4=[\ln(Z/Z-4)]/4 \tag{17}$$

showing that in two dimensions (but not three) $K_2=-K_4=\infty$, as expected.

Figure 3 shows the estimated critical exponent ν along the AIP and PB lines obtained from equations (8), (15) and (16) respectively. At the points P, I and $A(K_4\to\infty)$ we have $\nu_P=1.68$, $\nu_I=1.67$ and $\nu_A=0$ which should be compared to the exact values $\nu_P=\frac{2}{3}$, $\nu_I=1$ and $\nu_A=\frac{3}{2}$. As remarked before (Indekeu *et al* 1982) this simple approximation gives critical exponents which are generally less accurate than the critical couplings. The position of the PB line (as well the PC line) is not exactly known and information about critical exponents is less available. Within the present approach we obtain $\nu_B\to\nu_I$ at the point $B(K_4\to\infty)$ as expected. However, we notice a rather pathological behaviour for ν along the PB line close to the P point, which is probably connected to the assumption used to obtain equation (16). Such behaviour has also been seen in the study of the antiferromagnetic Ising model on the triangular lattice (Slotte 1984). No information about ν_4 (related to the coupling J_4) can be obtained with the present choice for the clusters along these lines once K_4' does not appear in the one-site cluster.

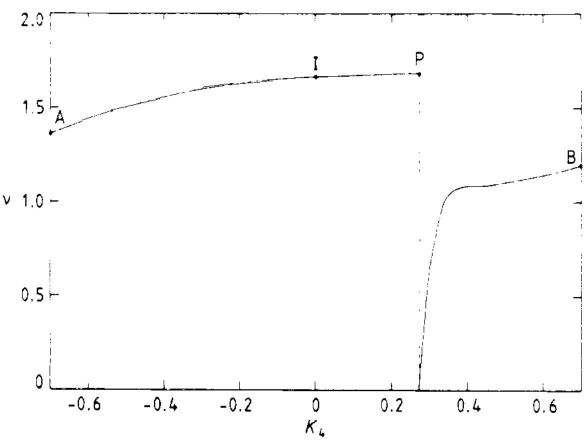

Figure 3. Critical exponent ν as a function of K_4.

In conclusion, the present approach has reproduced all the qualitative features of the phase diagram of the ATM. This is a consequence of the fact that the clusters used herein, even in their smallest sizes, carry all the basic symmetries of the model. This should also occur for bigger systems. We then expect that by considering bigger clusters all these features will be kept with just the improvement of the values of K_I and K_P, as well as the critical exponents. In fact, this is the case for the Ising model ($K_4 = 0$) (Indekeu *et al* 1982).

As a final remark, for $d = 3$ the main qualitative difference lies in the fact that the critical coupling $K_2 = -K_4$ is finite (see equation (17)). However, mean-field results (Ditzian *et al* 1980) show that the model has first-order transition lines, which are very difficult to obtain by the present approach.

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