

Large- N limit of the XY -Ashkin–Teller model: solution in two dimensions

G Gonnella and A Lamura

Istituto Nazionale per la Fisica della Materia (INFM) and Dipartimento di Fisica, Università di Bari and Istituto Nazionale di Fisica Nucleare, Sezione di Bari, via Amendola 173, 70126 Bari, Italy

Received 30 April 1999

Abstract. We introduce a vector model coupled to an N -colour Ashkin–Teller model and solve its phase diagram in the large- N limit in two dimensions. It is shown that the transition line starts from the axis of Ising couplings with a behaviour which can be critical or first order depending on the strength of the four-spin coupling and of the coupling between spin and vector variables. Below a negative value of the four-spin coupling the transition is always continuous.

The aim of this paper is to report results of the analytic study in the limit of infinite components of a model where vector spins are coupled to Ising variables in such a way that the vectors only interact inside each Ising domain. Models of this kind are expected to describe the critical behaviour of a class of systems with $O(2) \times Z_2$ ground-state symmetry which includes, for example, two-dimensional fully frustrated XY models [1]. The ground-state manifold of these models possesses discrete Ising-like chiral symmetry in addition to global continuous rotation symmetry in spin space and excitations consist of two types of stable topological defects: line defects of chiral domain walls and point defects, which are vortices. Physical systems described by the fully frustrated XY model are, for example, Josephson-junction arrays in a transverse magnetic field with $\frac{1}{2}$ flux per plaquette [2].

A prototype model with the above characteristics is the XY -Ising model defined by the Hamiltonian [3, 4]

$$H = -\beta^{-1} \sum_{\langle ij \rangle} [A \vec{n}_i \cdot \vec{n}_j (1 + s_i s_j) + C s_i s_j] \quad (1)$$

where $\beta^{-1} = K_B T$, the sum is over the nearest neighbours in a two-dimensional square lattice, $s_i = \pm 1$ is an Ising spin at the i -site and \vec{n}_i is a two-component unit vector at the i -site. The neighbouring vectors, \vec{n}_i, \vec{n}_j , interact with strength $2A$ only when the sites i, j are not separated by Peierls interfaces. The parameter C controls the amount of these interfaces. The phase diagram of the XY -Ising model has been studied by several methods [3–5]. At large values of C there is Ising order and the usual Kosterlitz–Thouless transition for the XY model has been observed. At smaller values of C Monte Carlo [3, 4] and Migdal–Kadanoff renormalization [5] results show that there is no phase with Ising disorder and XY order. This has been related [6] to the symmetry of the model under the transformation $\vec{n}_i \rightarrow s_i \vec{n}_i$, since the vectors \vec{n}_i are not coupled across an Ising domain wall where $s_i s_j + 1 = 0$. An interesting locus of the phase diagram of the model is the line where Ising and vector variables

simultaneously order. The critical exponents, associated with the Z_2 order parameter, have been found to vary systematically along this line which appeared to be non-universal [3]. Monte Carlo transfer matrix calculations [6] found no clear evidence for variation of these exponents, which, however, are significantly different from the pure Ising values.

In this paper we consider a convenient generalization of the the XY -Ising model defined by the partition function

$$Z = \sum_{\{s_i^\alpha = \pm 1\}} \int_{-\infty}^{+\infty} \prod_i d\bar{n}_i \delta\left(\frac{|\bar{n}_i|^2}{N} - 1\right) \times \exp\left\{\sum_{\langle ij \rangle} \left[A \bar{n}_i \cdot \bar{n}_j \left(1 + \frac{1}{N} \sum_{\alpha=1}^N s_i^\alpha s_j^\alpha\right) + C \sum_{\alpha=1}^N s_i^\alpha s_j^\alpha + \frac{D}{N} \left(\sum_{\alpha=1}^N s_i^\alpha s_j^\alpha\right)^2 \right]\right\} \quad (2)$$

where the couplings have been rescaled in order to get a sensible $N \rightarrow \infty$ limit. A term proportional to D which couples the different Ising species has been also introduced. For $A = 0$ and $N = 2$ the model has the same Hamiltonian of the Ashkin–Teller model [7], whose phase diagram in two dimensions in the large N limit was studied in [8]. In the following we will consider the model (2) in the $N \rightarrow \infty$ limit.

The constraints in the integral (2) can be recast by introducing the standard δ -function representation

$$\delta\left(\frac{|\bar{n}_i|^2}{N} - 1\right) = \frac{N}{2\pi} \int_{-\infty}^{+\infty} dz_i \exp\left\{-Nz_i \left(\frac{|\bar{n}_i|^2}{N} - 1\right)\right\} \quad (3)$$

where the integral is on the imaginary axis with $\text{Re } z$ arbitrary. After expressing the biquadratic terms in the Hamiltonian using the Hubbard–Stratanovich transformation, the partition function can be rewritten as

$$Z = \left(\frac{N}{2\pi}\right)^{N_0} \left(\sqrt{\frac{N}{2\pi A}}\right)^{2N_0} \left(\sqrt{\frac{N}{2\pi|2D-A|}}\right)^{N_0} \times \int_{-\infty}^{+\infty} \prod_i dz_i \int_{-\infty}^{+\infty} \prod_{\langle ij \rangle} d\zeta_{ij} \int_{-\infty}^{+\infty} \prod_{\langle ij \rangle} d\eta_{ij} \int_{-\infty}^{+\infty} \prod_{\langle ij \rangle} d\theta_{ij} \times \exp\left\{N \left[\sum_i z_i - \frac{1}{2A} \sum_{\langle ij \rangle} (\zeta_{ij}^2 - \eta_{ij}^2) - \frac{1}{2(2D-A)} \sum_{\langle ij \rangle} \theta_{ij}^2 - N_0 f_I(C + \zeta_{ij} + \theta_{ij}) - N_0 f_{SPH}(z_i; A + \zeta_{ij} + \eta_{ij}) \right]\right\} \quad (4)$$

where N_0 is the number of sites in the lattice, N_0 is the number of links, $f_I(C + \zeta_{ij} + \theta_{ij})$ is the Ising free energy per site in zero magnetic field with bond exchange energies $\{C + \zeta_{ij} + \theta_{ij}\}$ and

$$f_{SPH}(z_i; A + \zeta_{ij} + \eta_{ij}) = -\frac{1}{N_0} \ln \int_{-\infty}^{+\infty} \prod_i dn_i \exp\left(-\sum_i z_i n_i^2 + \sum_{\langle ij \rangle} (A + \zeta_{ij} + \eta_{ij}) n_i n_j\right). \quad (5)$$

We should observe that in (4) $\text{Re } \eta_{ij}$ is arbitrary and the integral in $d\theta_{ij}$ is on the real axis if $(2D - A) > 0$ or on the imaginary axis with $\text{Re } \theta_{ij}$ arbitrary if $(2D - A) < 0$. In the $N \rightarrow \infty$ limit the partition function can be evaluated by the steepest-descent method. Looking for

homogeneous solutions of the saddle-point equations $z_i = z \forall i$, $\zeta_{ij} = \zeta$, $\eta_{ij} = \eta$ and $\theta_{ij} = \theta \forall (i, j)$, the free energy per site and per component $f \equiv -\ln Z/NN_0$ reads as

$$f = -z + \frac{d}{2A}(\zeta^2 - \eta^2) + \frac{d}{2(2D - A)}\theta^2 + f_I(C + \zeta + \theta) + f_{SPH}(z; A + \zeta + \eta) \quad (6)$$

where d denotes the number of spatial dimensions. The saddle-point equations $\partial f/\partial z = 0$, $\partial f/\partial \zeta = 0$, $\partial f/\partial \eta = 0$ and $\partial f/\partial \theta = 0$ are

$$1 = \frac{\partial f_{SPH}(z; A + \zeta + \eta)}{\partial z} \quad (7)$$

$$\frac{d\zeta}{A} = -\frac{\partial f_{SPH}(z; A + \zeta + \eta)}{\partial \zeta} - \frac{\partial f_I(C + \zeta + \theta)}{\partial \zeta} \quad (8)$$

$$\frac{d\eta}{A} = \frac{\partial f_{SPH}(z; A + \zeta + \eta)}{\partial \eta} \quad (9)$$

$$\frac{d\theta}{2D - A} = -\frac{\partial f_I(C + \zeta + \theta)}{\partial \theta}. \quad (10)$$

Here the arbitrariness of $\text{Re } \eta$ (and of $\text{Re } \theta$ if $2D - A < 0$) is used for satisfying the above equations with $\text{Im } \eta = 0$ (and $\text{Im } \theta = 0$ if $2D - A < 0$). From now on we will restrict our discussion to the case with $d = 2$. Introducing the variable $x = \tanh(C + \zeta + \theta)$ and using the explicit expression of $f_I(C + \zeta + \theta)$ [9], the saddle-point equation (10) can be written as

$$\tanh^{-1} x = C + \zeta + \frac{2D - A}{2} F(x) \quad (11)$$

with

$$F(x) = \frac{1}{2} \left\{ x + \frac{1}{x} + \frac{2}{\pi} K_1(k) \left[k(1 + x^2) - \frac{1 - 3x^2}{x} \right] \right\} \quad (12)$$

where $k = 4x(1 - x^2)/(1 + x^2)^2$ and $K_1(k)$ is the complete elliptic integral of the first kind. We can now express equation (11) in terms of x only, using equations (7)–(9):

$$\tanh^{-1} x = C + DF(x) - \frac{1}{2(2 + F(x))} \left\{ 1 - 2A \left(1 + \frac{F(x)}{2} \right) \left[\Psi_2^{-1} \left(2A \left(1 + \frac{F(x)}{2} \right) \right) + 2 \right] \right\} \quad (13)$$

with

$$\Psi_2(\xi) = \frac{1}{N_0} \sum_{\vec{q}} \frac{1}{2 - \sum_{\mu=1}^2 \cos q_\mu + \xi} \quad (14)$$

where the sum in \vec{q} is over the first Brillouin zone in the reciprocal lattice, having used the fact that

$$f_{SPH}(z; A + \zeta + \eta) = \frac{1}{2N_0} \sum_{\vec{q}} \ln \left[z - (A + \zeta + \eta) \sum_{\mu=1}^2 \cos q_\mu \right] - \frac{1}{2} \ln \pi. \quad (15)$$

No transition is obtained for the sub-system described in terms of the \vec{n}_i variables [10] due to the fact that we are in $d = 2$. Following [8], we solved equation (13) for $x \sim x_0 = \sqrt{2} - 1$, that is to say near the Ising solution. By setting $x = x_0 - \delta$, equation (13) reads as

$$0 \simeq \sigma + \Lambda \delta + \Xi \delta \ln |\delta| \quad (16)$$

where

$$\begin{aligned}\sigma &= \sqrt{2}D + C + A + \frac{A}{2}\Psi_2^{-1}\left[2A\left(1 + \frac{\sqrt{2}}{2}\right)\right] - \frac{1}{2}\ln(1 + \sqrt{2}) - \frac{1}{2(2 + \sqrt{2})} \\ \Lambda &= \frac{\sqrt{2} + 1}{2}\left\{1 + 2(\Delta + D) - \frac{8}{\pi}(\Delta + D)\ln[2\sqrt{2}(\sqrt{2} - 1)]\right\} \\ \Xi &= \frac{4}{\pi}(1 + \sqrt{2})(\Delta + D)\end{aligned}$$

with

$$\Delta = \frac{1}{2(2 + \sqrt{2})^2} + \frac{A^2}{2}(\Psi_2^{-1})'\left[2A\left(1 + \frac{\sqrt{2}}{2}\right)\right]. \quad (17)$$

$(\Psi_2^{-1})'$ in (17) indicates the derivative of the function Ψ_2^{-1} . It is straightforward to prove that in the limit $A \rightarrow 0$ one recovers the results obtained by Fradkin in [8]. Indeed, Ψ_2^{-1} can be expanded at small ξ as [11]

$$\Psi_2^{-1}(\xi) = \frac{1}{\xi}\left[1 - 2\xi + \xi^2 + \frac{\xi^4}{4} + o(\xi^6)\right] \quad (18)$$

so that σ tends to the value $\sqrt{2}D + C - \frac{1}{2}\ln(1 + \sqrt{2})$ and, from equation (17), it transpires that

$$\Delta = \frac{A^2}{2} + o(A^4). \quad (19)$$

Setting $\sigma = 0$ (i.e., on the phase boundary [8]) we find the solutions

$$\delta = 0 \quad (20)$$

$$\delta = \pm e^{-\Lambda/\Xi} = \pm[2\sqrt{2}(\sqrt{2} - 1)]e^{-\pi/4}e^{-\pi/8(\Delta+D)}. \quad (21)$$

The nature of the transition depends on the sign of $(\Delta + D)$. For $(\Delta + D) > 0$ both (20) and (21) are solutions, with the double root being the stable solutions which minimize the free energy. For $(\Delta + D) < 0$, at $\sigma = 0$ the only solution is $\delta = 0$, which corresponds to the usual critical transition, while for $\sigma \neq 0$ but small, there is a nonlinear relation between δ and σ [8]. The critical behaviour near the Ising solution is similar to that obtained by Fradkin for the large N -limit of the Ashkin–Teller model [8]. In [8] the critical behaviour depends on the sign of the four-spin coupling constant (D in our model): the transition is first order for positive values of the four-spin coupling constant and second order for negative values. In our model the critical behaviour is controlled by the sign of the quantity $(\Delta + D)$. In order to describe the behaviour of the transition line we show in figure 1 the plot of Δ as a function of A . It can be seen from figure 1 that Δ increases up to a maximum value Δ_M which is approximately 0.043, located at $A \simeq 0.52$, and then decreases, becoming zero at $A \simeq 7.09$. Thus we expect the following behaviour in the C – A coupling constant plane:

- (1) $D \geq 0$. The transition line, defined by $\sigma = 0$, starts from the C -axis at small positive A with a first-order behaviour, then it becomes continuous at a tricritical point ($\Delta + D = 0$). In the special case $D = 0$, the point on the C -axis at $A = 0$ is a tricritical point since $\Delta + D = 0$.
- (2) $-\Delta_M \leq D < 0$. The transition line has a second-order behaviour for small values of A , then at a tricritical point it becomes first order up to a second tricritical point, where the transition again becomes continuous. The range of values of A for which the transition is first order reduces as $D \rightarrow -\Delta_M$, and the two tricritical points coalesce in a single point when $D = -\Delta_M$.

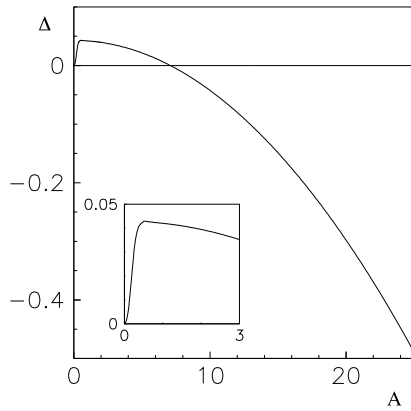


Figure 1. The plot of Δ as function of A . For a better view, in the inset Δ is plotted in a smaller range of values of A .

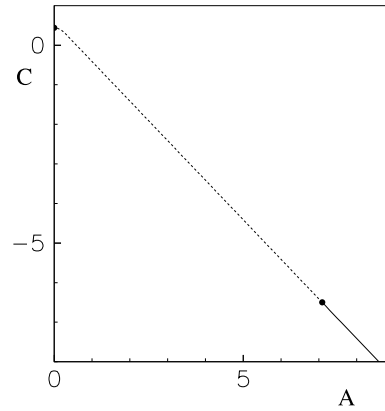


Figure 2. The phase diagram of the model with $D = 0$. The full and broken lines represent the continuous and first-order transition, respectively. Filled circles indicate the positions of tricritical points.

(3) $D < -\Delta_M$. The transition line is always continuous since $(\Delta + D) < 0 \forall A$.

We numerically solved the equation $\sigma = 0$ for different values of D . The phase boundary for the case $D = 0$ is shown in figure 2. A transition line starts from a tricritical point on the C -axis, as previously explained, with a first-order behaviour ($(\Delta + D) > 0$). The Ising transition point ($C/K_B T = \frac{1}{2} \ln(1 + \sqrt{2}) \simeq 0.44$ [12]) is correctly recovered in the limit $A \rightarrow 0$ as one expects. At $A \simeq 7.09$, $C \simeq -6.50$ there is a second tricritical point, where the transition line becomes second order ($(\Delta + D) < 0$). This behaviour is quite different from that found by Monte Carlo simulations for the XY -Ising model [4]. In that case the transition line starts from the axis of Ising couplings with a continuous character which becomes first order at a tricritical point at $A \simeq 3-5$, $C \simeq -4.3$. Moreover, Monte Carlo simulations found the XY transition line, which intersects the other transition line (corresponding to the one shown in figure 2) at $A \simeq 0.6$, $C \simeq 0.15$. Actually, a strict comparison between our phase diagram and Monte Carlo results cannot be done since in our approximation the ordered phase for the vector variables cannot be found. It is interesting to observe that a boundary can be established for the region of the phase diagram which contains the transition line. Indeed, for the general properties of the function $\Psi_2(\xi)$ [13], the function $\Psi_2^{-1}(\xi)$ is positive for ξ positive. This fact can be used to determine the coupling constant space where the equation $\sigma = 0$ can be fulfilled. Using the expression of σ and equating it to zero, it is straightforward to show that for positive values of A , there exists an upper bound C_{sup} for the critical value of the coupling constant C , given by the equation

$$C_{sup} = \frac{1}{2} \ln(1 + \sqrt{2}) + \frac{1}{2(2 + \sqrt{2})} - A - \sqrt{2}D. \tag{22}$$

We find numerically that the transition line of the phase diagram tends asymptotically in the limit $A \rightarrow \infty$ to the straight line defined by the equation (22).

The phase diagram for the case $D = -0.03$ is reported in figure 3. A second-order line starts from the C -axis with a value $C \simeq 0.483$, which is different from the Ising transition point because the coupling constant D changes the effective bond strength for the Ising spins. Then, the critical line becomes first order at the tricritical point which occurs at $C \simeq 0.38$, $A \simeq 0.24$. A second tricritical point is located at $C \simeq -3.25$, $A \simeq 3.88$, where the transition line again

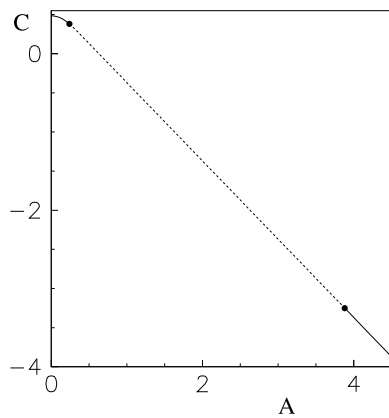


Figure 3. The phase diagram of the model with $D = -0.03$. The full and broken lines represent the continuous and first-order transition, respectively. Filled circles indicate the positions of tricritical points.

becomes second order. Also in this case we observe that the transition line tends asymptotically to the straight line defined by equation (22).

It would be interesting to extend this analysis to $d = 3$, where one expects an ordered phase for the \vec{n}_i variables in the $N \rightarrow \infty$ limit [10]. At the same time it would be an important endeavour to deduce a realistic picture of the model (2) beyond the $N \rightarrow \infty$ approximation.

In summary, we have studied the phase diagram of an N -vector model coupled to an N -colour Ashkin–Teller model in the $N \rightarrow \infty$ limit in two dimensions. The resulting phase diagrams are shown in figures 2 and 3 for two values of the four-spin coupling constant. They show a transition line starting from the axis of Ising couplings whose behaviour depends on the sign of quantity $(\Delta + D)$. We find that there is a negative value of D below which the transition is continuous.

References

- [1] Villain J 1977 *J. Phys. C: Solid State Phys.* **10** 4793
See also the bibliography in [4]
- [2] Teitel S and Jayaprakash C 1983 *Phys. Rev. B* **27** 598
Teitel S and Jayaprakash C 1983 *Phys. Rev. Lett.* **51** 199
- [3] Granato E, Kosterlitz J M, Lee J and Nightingale M P 1991 *Phys. Rev. Lett.* **66** 1090
- [4] Lee J, Granato E and Kosterlitz J M 1991 *Phys. Rev. B* **44** 4819
- [5] Granato E 1987 *J. Phys. C: Solid State Phys.* **20** L215
- [6] Nightingale M P, Granato E and Kosterlitz J M 1995 *Phys. Rev. B* **52** 7402
- [7] Ashkin J and Teller E 1943 *Phys. Rev.* **64** 178
- [8] Fradkin E 1984 *Phys. Rev. Lett.* **53** 1967
- [9] Huang K 1987 *Statistical Mechanics* (New York: Wiley)
- [10] Berlin T H and Kac M 1952 *Phys. Rev.* **86** 821
Stanley H E 1968 *Phys. Rev.* **176** 718
- [11] Ohno K, Carmesin H O, Kawamura H and Okabe Y 1990 *Phys. Rev. B* **42** 10 360
- [12] See, for example, Domb C 1974 *Phase Transitions and Critical Phenomena* ed C Domb and M S Green (London: Academic)
- [13] See, for example, Baxter R J 1982 *Exactly Solved Models in Statistical Mechanics* (London: Academic)