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1984 J. Phys. A: Math. Gen. 17 1913

(http://iopscience.iop.org/0305-4470/17/9/025)

J. Phys. A: Math. Gen. **17** (1984) 1913–1920. Printed in Great Britain

Renormalisation-group study of crossover behaviour in an extended ϕ^4 model on a square lattice

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Received 28 June 1983, in final form 1 December 1983

Abstract. A real-space renormalisation-group transformation is applied to study the order–disorder-displacive crossover in a ϕ^4 lattice model involving some nearest-neighbour and next-nearest-neighbour interactions. A non-trivial fixed point is found on the crossover surface. It is shown that the point is associated with a 'true' critical behaviour of the system. This critical behaviour is suggested to be a consequence of a continuous phase transition from a phase characterised by the appearance of locally ordered clusters and a long-range order between them to a more disordered high-temperature phase in which the clusters disappear.

1. Introduction

The ϕ^4 model on a lattice has been used in recent years to study some static and dynamic properties of systems undergoing structural phase transitions. The static renormalisation-group (RG) analysis of the behaviour of two-dimensional ϕ^4 systems shows that their phase diagram can be divided into three regions, namely, an ordered phase, a disordered Ising-like region, and a Gaussian-like region. The division of the parameter space into the three regions is essentially the same for different parametrisations (Bruce and Schneider 1977, Burkhardt and Kinzel 1979, Beale *et al* 1981, Baker *et al* 1982). The disordered Ising-like and Gaussian-like regions are separated by the so-called crossover line. Points on the crossover line flow under the RG transformation to a high-temperature fixed point. The ordered and disordered Ising-like regions are separated by a critical line and points on this line are driven by the RG transformation toward the Ising fixed point. Within the ordered phase as well as the disordered Ising-like region the renormalised one-point potential exhibits near the Ising limit a double-well structure, whether the original one-point potential has double-well (order–disorder regime) or single-well (displacive regime) character. Thus, close to the Ising limit, especially near the critical region, the coordinates of a renormalised displacive model reveal a behaviour qualitatively similar to that of the coordinates of an order–disorder model. This implies that the structural phase transitions have always order–disorder character in two dimensions and the essential difference between the two (displacive and order–disorder) categories of systems undergoing structural phase transitions appears to be a matter of length scales (Bruce 1978, Bruce *et al* 1979). Moreover, systems undergoing structural phase transitions are in the same universality class as the Ising model (Beale *et al* 1981).

Results of the molecular-dynamics studies of systems exhibiting structural phase transitions give strong evidence of the formation of locally ordered domains or clusters,

0305-4470/84/091913+08$02.25

separated by cluster walls (solitons), over a wide range of temperatures from temperatures close to but below the critical temperature (Schneider and Stoll 1973, 1976, Schneider 1977). The very appearance of such clusters is accompanied by the presence of a double well in the effective one-particle potential, i.e. the real-site potential which is felt by each particle. Consequently, the fluctuations in the local order parameter can have two distinct time scales, namely, the short time scale associated with the relatively fast collective phonon-like oscillations around displaced or non-displaced instantaneous mean positions and the long time scale connected with the collective inter-well hopping. The occurrence of the collective motion of the second kind and the formation of locally ordered clusters is possible only if the effective site potential has a double-well structure. Such a structure can occur for order–disorder as well as for displacive models but its appearance is dependent on temperature. It turns out that above a certain temperature, called the crossover temperature T_I, the system has no possibility of a spontaneous symmetry breaking and the effective one-point potential can have only the single-well character. It should be pointed out that T_I is not the temperature T_0 introduced earlier (Beale *et al* 1981). The latter is a temperature of the non-critical crossover between two different kinds of the RG flow and, being a function of the parameters of the Hamiltonian, refers to each point on the crossover line in the parameter space. In turn, the temperature T_I is connected to the fixed point of a RG transformation and appears to be a temperature of a continuous phase transition. At this temperature the system passes to a phase in which clusters disappear.

The existence of only short-range ordered clusters below this temperature (but above the temperature of the structural phase transition T_c) does not mean, however, that within this temperature range there is no long-range order and no phase transition. Since each cluster acts in principle as a 'superparticle' one can expect the occurrence of a long-range order associated with the correlations between clusters. Indeed, the RG analysis of the shape of the renormalised one-particle potential shows that the appearance of the double-well structure of the effective site potential, and hence the existence of locally ordered clusters, is due to the correlations of particles at sufficiently long distances (Beale *et al* 1981). When temperature increases up to T_I, the range of the correlations, which play an essential role in forming the double-well structure of the effective one-point potential, tends to infinity. Thus, the occurrence of locally ordered clusters near T_I is caused by very long-ranged particle correlations. Accordingly, there are long-range correlations between clusters and at T_I the range of the correlation of superparticle (cluster) fluctuations should diverge. The existence of the long-range order between clusters can also be explained as follows. The long-range order between particles occurs in ϕ^4 systems if the well depth of the effective one-particle double-well potential is sufficiently large compared with the particle thermal energy. Obviously, this condition is not satisfied for temperatures $T > T_c$ and the long-range order between particles does not appear. However, the well depth of the effective cluster potential, i.e. the potential barrier seen by the cluster during the inter-well hopping, is directly proportional to the number of particles of which the cluster consists. One can therefore expect that even above T_c the well depth of the effective cluster potential is very large compared with the cluster thermal energy. In such a case clusters behave in the temperature range $T_c < T < T_I$ in a similar way to simple particles below T_c. This suggests that below T_I there should occur a long-range order between clusters, although there is no long-range order due to correlations between simple particles. Obviously, the probabilities of the existence of two identical clusters but with opposite signs of the local order parameter are the same for $T_c < T < T_I$

and the long-range order between clusters can have only an 'antiferromagnetic' or 'antiferroelectric' character. This long-range order vanishes when the temperature T_I is approached since at T_I clusters become unstable and decay. Then, the order–disorder-to-displacive crossover at T_I can be considered as a continuous phase transition. In this paper we apply a real-space RG method to study the behaviour of an extended ϕ^4 model near T_I. We find a singly unstable (with respect to temperature) fixed point corresponding to T_I and determine numerically the critical exponents ν and η.

2. The model and the RG transformation

It has been shown that the two-parameter space usually used for the RG analysis of the ϕ^4 model is not capable of yielding a correct and complete description of the behaviour of the system near the crossover region. Above all, the two-parameter RG approach leads to a Gaussian-like symmetry of the fixed point associated with T_I and gives an infinite value for T_I (Beale *et al* 1981, Baker *et al* 1982, Baker and Bishop 1982). Thus, to obtain a more realistic description of the system near T_I one has to enlarge the parameter space, i.e. one has to take into account some additional interactions. Accordingly, we consider here the following Hamiltonian on a square lattice

$$-\frac{H\{x_i\}}{k_B T} = a_1 \sum_{i=1}^{N} x_i^2 - a_2 \sum_{i=1}^{N} x_i^4 + K_1 \sum_{\langle i,j\rangle} x_i x_j + K_2 \sum_{\langle i,j\rangle} (x_i^3 x_j + x_i x_j^3) + K_3 \sum_{\langle i,j\rangle} x_i^2 x_j^2 + L_1 \sum_{(i,j)} x_i x_j + L_2 \sum_{(i,j)} (x_i^3 x_j + x_i x_j^3) + L_3 \sum_{(i,j)} x_i^2 x_j^2 \tag{2.1}$$

with $\{x_i\}$ being the displacements of a set of particles, the summation running over the N lattice points, and the symbols $\langle i, j\rangle$ and (i, j) denoting nearest-neighbour and next-nearest-neighbour pairs. It should be noted that the model described by the Hamiltonian (2.1) does not necessarily exhibit Gaussian-like symmetry at infinite-temperature fixed points. Indeed, it was proven that the lattice models for which the Hamiltonians satisfy the FKG inequalities (Fortuin *et al* 1971) always display the Gaussian-type symmetry at infinite-temperature fixed points of a block-variable RG (Baker and Krinsky 1977, Newman 1980). However, the FKG inequalities hold whenever the following conditions are fulfilled (Battle and Rosen 1980):

$$\partial^2 \mathcal{H}\{x_i\}/\partial x_i\, \partial x_j > 0, \qquad \forall i, j\ (i \neq j) \tag{2.2}$$

where $\mathcal{H}$ denotes the Hamiltonian of a given lattice system. It can be easily verified that the conditions (2.2) are not in general satisfied for the Hamiltonian (2.1) because the variables x_i take on values from $-\infty$ to $+\infty$. Thus, our model, in contrast to the ordinary ϕ^4 model, does not necessarily reduce to a Gaussian model at high-temperature fixed points.

In the analysis of the behaviour of the system near the crossover fixed point, i.e. the fixed point related to the crossover temperature T_I, we shall apply a lattice-space RG method which consists of the decimation transformation and a variable rescaling. The RG transformation associated with this method can be defined by

$$E - \frac{H'\{y_i'\}}{k_B T} = \left\{ \ln\left[\int_{-\infty}^{+\infty} \prod_i \mathrm{d}x_i \prod_{i \in \mathcal{S}_1} [\delta(x_i - y_i)] \exp\left(-\frac{H\{x_i\}}{k_B T}\right)\right]\right\}_{y_i \to s y_i'}, \tag{2.3}$$

where E is a constant, and s denotes a variable rescaling factor which will be related

to the length rescaling factor b. The y_i' stand for new variables distributed on a new lattice, isomorphic to the original one, whose points belong to a subset $\mathcal{S}_1$ of the entire set of initial lattice points. As long as the factor s is not determined, the transformation (2.3) yields a line of fixed points (Bell and Wilson 1975), and to allow the method to be utilised one has to find a criterion for choosing the factor s. Such a criterion cannot however be found in a quite accurate and unambiguous manner. We note that the transformation (2.3) together with a suitable procedure for determining the factor s was used to describe the critical behaviour of a continuous-variable Ising model on a square lattice (Jeżewski 1980, 1983). Since in this paper we are concerned with the behaviour of the system near the crossover fixed point, we can select the rescaling factor in such a way that the transformation (2.3) could have the crossover fixed point, i.e. the fixed point at which $a_1^* = 0$. In the light of earlier investigations (Beale *et al* 1981) the crossover fixed point should really exist.

The numerical calculations for the Ising-like critical fixed point suggest that, as far as the transformation (2.3) is concerned, long-range and complex interactions are of minor importance compared with the interactions included in the Hamiltonian (2.1) (Jeżewski 1983). Therefore, the Hamiltonian (2.1) is expected to be also adequate for discussing the behaviour of the system near the crossover fixed point.

3. Critical behaviour at the temperature T_1

In applying the RG transformation (2.3) to the Hamiltonian (2.1) we employ here the cumulant expansion procedure (Niemeijer and van Leeuwen 1976). Accordingly, we split the Hamiltonian (2.1) into one-site terms (treated as a zeroth part) and multi-site terms or interactions (perturbational part). As can be easily shown, the first-order cumulant approximation is not good enough to provide a reliable analysis of the behaviour of the system near the crossover fixed point. The lowest-order approximation which can be considered as quite sensible is the cumulant expansion to second order in the interaction parameters. The RG equations in the second-order approximation are found for the case of $b = \sqrt{2}$ to be

$$a_1' = s^2[a_1 + 4I_2K_3 + 2I_2K_1^2 + 4I_4K_1K_2 + 2I_6K_2^2 + 16(I_2I_4 - I_2^3)K_3L_3], \tag{3.1}$$

$$a_2' = s^4[a_2 - 4I_2K_1K_2 - 4I_4K_2^2 - 2(I_4 - I_2^2)K_3^2], \tag{3.2}$$

$$K_1' = s^2(L_1 + 2I_2K_1^2 + 4I_4K_1K_2 + 2I_6K_2^2), \tag{3.3}$$

$$K_2' = s^4(L_2 + 2I_2K_1K_2 + 2I_4K_2^2), \tag{3.4}$$

$$K_3' = s^4[L_3 + 2(I_4 - I_2^2)K_3^2], \tag{3.5}$$

$$L_1' = s^2(I_2K_1^2 + 2I_4K_1K_2 + I_6K_2^2), \tag{3.6}$$

$$L_2' = s^4(I_2K_1K_2 + I_4K_2^2), \tag{3.7}$$

$$L_3' = s^4(I_4 - I_2^2)K_3^2, \tag{3.8}$$

with

$$I_n = a_2^{-n/4} \int_{-\infty}^{+\infty} \mathrm{d}x\, x^n \exp(gx^2 - x^4) \Big/ \int_{-\infty}^{+\infty} \mathrm{d}x \exp(gx^2 - x^4) \tag{3.9}$$

where $g = a_1/\sqrt{a_2}$. It is remarkable that the use of the non-Gaussian distributions in

deriving the above recursion relations does not involve the necessity of applying any approximations in further calculations. Indeed, for a given fixed point, equations (3.1), (3.2) and (3.3) can be cast in the form

$$g^* = \frac{2s^2}{1-s^2}\left[2\left(4+\frac{1}{s^4(2+s^4)}\right)\frac{v}{w-v^2}+\frac{1}{s^2(2+s^2)}\tilde{K}_1^*\right], \tag{3.10}$$

$$1 = 2s^4\left[1-\frac{1}{s^4(2+s^4)}\left(\frac{2}{w}+\frac{1}{w-v^2}\right)+\frac{2}{s^4(2+s^4)}\frac{v}{w}\tilde{K}_1^*\right], \tag{3.11}$$

$$\tilde{K}_1^* = s^2(2+s^2)\left(\frac{f}{s^8(2+s^4)^2}+\frac{2}{s^4(2+s^4)}(1-vf)\tilde{K}_1^*-v(1-vf)(\tilde{K}_1^*)^2\right), \tag{3.12}$$

with

$$vg^* = 2w-\tfrac{1}{2}, \tag{3.13}$$

$$f = (\tfrac{3}{4}v+\tfrac{1}{2}g^*w)/w^2, \tag{3.14}$$

where $\tilde{K}_1^* = K_1^*/\sqrt{a_2^*}$, $v = \sqrt{a_2^*}\, I_2^*$ and $w = a_2^* I_4^*$. The solution of (3.10), (3.11) and (3.12) gives the fixed-point values of the parameters a_1, a_2 and K_1. Fixed-point values of other parameters can be expressed by a_1^*, a_2^* and K_1^*. On solving (3.10), (3.11) and (3.12) one arrives at a cubic equation for w with the coefficients being functions of the factor s. The numerical calculations show that for the case of the length rescaling factor $b = \sqrt{2}$ and for values of variable rescaling factor in the range $0 \leqslant s \leqslant 1$ the RG equations have only one crossover fixed point, namely,

$$a_1^* = a_2^* = K_\alpha^* = L_\alpha^* = 0, \qquad \alpha = 1, 2, 3, \qquad s = 0.952. \tag{3.15}$$

This point is singly unstable and lies on a surface of attraction which by analogy to earlier investigations (Beale *et al* 1981) may be called the crossover surface. It must be stressed that the temperature T_1 associated with the fixed point (3.15) is not necessarily infinite, as points on the crossover surface correspond in general to various systems described by the Hamiltonian (2.1) and thus to various values of T_1. Then, the existence of the fixed point (3.15) can be connected to a continuous phase transition at finite temperature. The vanishing of the renormalised potential at the crossover fixed point bears a resemblance to the behaviour of the effective potential of a sine-Gordon system at the 'unlocking' transition (Puga *et al* 1982). However, studies of the thermodynamic properties of kinks in one-dimensional continuum ϕ^4 and sine-Gordon systems suggest that the shape of the renormalised potential depends strongly on the parametrisation of the system (Maki and Takayama 1979, Takayama and Maki 1979). Thus, one can expect that on extending the Hamiltonian (2.1) to include additional couplings, or on extending the calculations to a fairly high order of the cumulant expansion, it would be possible to obtain a crossover fixed point for which $a_2^* \neq 0$, $K_\alpha^* \neq 0$ and $L_\alpha^* \neq 0$ ($\alpha = 1, 2, 3$). It is to be noted that the phase transition at T_1 can be interpreted as a crossover from a low-temperature symmetry broken state to a high-temperature symmetric state, already known in field theory (Amit 1978, Brout and Deans 1983, Callaway and Maloof 1983).

The definition of the order parameter, vanishing at T_1, is in a sense a matter of choice. One of the most natural ways to choose the order parameter is

$$\psi = \sum_{l=2}^{\infty}\sum_{k=1} k[p_l^+(T)+p_l^-(T)] \tag{3.16}$$

where $p_l^+(T)$ and $p_l^-(T)$ denote the probabilities of the occurrence of clusters with l particles in a unit volume and at a given temperature T. The superscripts + and − refer to two different directions in which the particles can be displaced. We remark that the least cluster consists of two particles. The dependence of the probabilities p on temperature is such that $p_l^+(T)>0$ and $p_l^-(T)>0$ below T_1 (for each $l\geq 2$) and $p_l^+(T)=p_l^-(T)=0$ above T_1. Obviously, $p_l^+(T)\neq p_l^-(T)$ below T_c and $p_l^+(T)=p_l^-(T)$ for $T_c<T<T_1$. The above features of the probabilities p reflect thermodynamic properties of clusters exhibited by computer simulations. The probabilities p do not yield, however, any detailed information concerning the topology and the shape of clusters. We notice that it would also be possible to define the order parameter taking into account the average size of clusters. Indeed, above T_c the average size of clusters decreases and vanishes at T_1. This also implies that the probability of the existence of large clusters decreases more rapidly than the probability of the existence of small clusters, as the temperature approaches T_1.

The increase of temperature is accompanied for $T\leq T_1$ by the enlargement of the range of particle correlations, being of essential importance for the formation of the double-well structure of the effective one-point potential and thereby for the formation of locally ordered clusters. Thus, one can infer that clusters are strongly correlated with each other. These clusters, due to their stability, can be treated as long-lifetime superparticles. We notice that besides clusters, there are in the system also simple particles which do not belong to any cluster. The difference in the thermodynamic behaviour of clusters and simple particles appears to rely on the fact that the collective inter-well motions of clusters are associated with a very long time scale compared with fast motions of simple particles. In other words, clusters behave as superparticles with large masses in comparison with masses of simple particles. Then, the range of the correlation of fluctuations connected with interactions between single particles and clusters, similarly to the range of the correlation of single-particle fluctuations, does not tend to infinity above T_c. However, the barriers which encounter clusters during the inter-well motions can be very large compared with their thermal energies, and in consequence clusters can reveal in the temperature range $T_c<T<T_1$ a similar behaviour to simple particles below T_c. One can therefore expect that when the temperature grows up to T_1 the range of the correlation of cluster fluctuations diverges and there is a long-range order associated with the existence of clusters and interactions between them. Since $p_l^+(T)=p_l^-(T)$ for $T_c<T<T_1$, such an order has an 'antiferromagnetic' or 'antiferroelectric' character.

The correlations between clusters can be described by the function

$$g_{\mathrm{cl}}(r)=\langle x_i x_{i+r}\rangle \tag{3.17}$$

where r is the distance (expressed in units of the lattice constant) between two given particles and cl denotes that these two particles belong to two different clusters. When $r\to\infty$ and $T\to T_1$ one can assume that the correlation function decays algebraically, i.e. for two-dimensional lattices one has

$$g_{\mathrm{cl}}(r)\sim r^{-\eta}. \tag{3.18}$$

The critical exponent η can be found from the relation (Jeżewski 1980)

$$s=b^{-\eta/2}. \tag{3.19}$$

Then, for the crossover fixed point (3.15) we obtain $\eta=0.284$. We note that, according to (3.18) and (3.19), the restriction of s to the range $0\leq s\leq 1$ we have adopted above

appears to be quite appropriate. Near T_I, the range of the correlation of cluster fluctuations is expected to be given by

$$\xi \sim |T - T_I|^{-\nu}. \tag{3.20}$$

The calculation of the critical exponent ν can be performed by standard methods (Niemeijer and van Leeuwen 1976). After having used the recurrence relation

$$\tilde{I}_{n+4} = \tfrac{1}{4}(n+1)a_2\tilde{I}_n + \tfrac{1}{2}g\sqrt{a_2}\,\tilde{I}_{n+2}, \qquad n = 0, 1, 2, \ldots, \tag{3.21}$$

one can show that the crossover fixed point is unstable only in the temperature direction with the critical exponent $\nu = 1.010$. It is rather striking that the indices ν and η are close to the Ising indices $\nu_{\text{Ising}} = 1$, $\eta_{\text{Ising}} = 0.25$. One would suppose that the exact values of the critical exponents associated with the crossover fixed point are identical with those related to the fixed point which corresponds to the structural phase transition, although these two fixed points are located at quite different places of the parameter space. It must be emphasised that the temperature T_I does not have to be infinite and the crossover fixed point can be accompanied by a 'true' continuous phase transition at a finite temperature.

4. Concluding remarks

We have employed a real-space RG method for studying the behaviour of a two-dimensional lattice system near the crossover temperature T_I, at which there occurs a changeover from double-well structure of the effective potential to single-well structure. The temperature T_I has been proven to be connected to a fixed point, unstable in the temperature direction. The critical exponents associated with this fixed point have been found to be close to the Ising indices. One then can conclude that at T_I there occurs a continuous phase transition, which can be interpreted as a transition from a phase characterised by the existence of locally ordered clusters and by long-range order between them to a fully disordered phase. Obviously, the interpretation presented in this paper cannot be strongly supported by the RG analysis. It should be also noted that the RG analysis carried out in this paper is not complete because it does not include the investigation of the flow diagram. However, the examination of the flow diagram for the case of the eight-parameter Hamiltonian seems to be a very laborious problem. It would also be interesting to extend the above considerations to the case of three dimensions. There is experimental evidence that the temperature of the structural phase transition T_c and the crossover temperature T_I coincide for some ferroelectric perovskite systems (Müller *et al* 1982).

Acknowledgments

The author would like to acknowledge helpful discussions with Dr Piotr Pierański. This work was supported by the Polish Academy of Sciences under project MR-I.9.

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