Order-disorder displacive crossover in a structural phase transition model

1982 J. Phys. A: Math. Gen. 15 L201

(http://iopscience.iop.org/0305-4470/15/4/009)

J. Phys. A: Math. Gen. 15 (1982) L201–L206. Printed in Great Britain

LETTER TO THE EDITOR

Order–disorder displacive crossover in a structural phase transition model†

George A Baker Jr and A R Bishop

Theoretical Division, Los Alamos National Laboratory, University of California, Los Alamos, NM 87545, USA

Received 16 November 1981

Abstract. We are able to write the partition function of the double-Gaussian model which is representative of the $\lambda\phi^4$ class (Hamiltonians with unbounded doubly degenerate local potentials) exactly as the product of the partition function of a Gaussian model and the partition function of a spin-$\frac{1}{2}$ Ising model. On the basis of this result we are able to determine the nature and location of the critical points of this model. It also follows that the block spin renormalisation group flows in the entire high-temperature region converge to a Gaussian model fixed point.

There have been several discussions (Beale *et al* 1981, Bruce 1980, Bruce and Schneider 1977, Bruce *et al* 1979, Schneider and Stoll 1980) of $\lambda\phi^4$ (double-well) models appropriate to structural phase transitions which have emphasised so-called displacive–order–disorder crossover. Generically, this crossover is proposed to occur at temperatures $\sim T_x(\theta) > T_c(\theta)$, where T_c is an (Ising) critical temperature and θ a parameter measuring the 'displaciveness' of the $\lambda\phi^4$ model (see below). At $T > T_x$, large-amplitude phonon-like modes (often characterised as 'displacive') are the dominant excitations, whereas for $T < T_x$ it is supposed that ordered domains (clusters) (and domain walls) dominate (characteristic of order–disorder models), and that the transition at $T_c(\theta)$ is continuous and belongs to the Ising universality class for *all* θ. Regimes of precursive order–disorder behaviour appear sufficiently near T_c no matter how displacive the bare Hamiltonians. This behaviour is consistent with *dynamic* structure factor observations in molecular dynamics simulations‡ (Bruce *et al* 1979, Schneider and Stoll 1980). For $T \leqslant T_x(\theta)$ an additional central (i.e. low-frequency) component in the structure factor is associated with cluster (domain) dynamics. This dynamic crossover is certainly *not* a sharp transition, but specific criteria for $T_x(\theta)$ from *static* properties have been proposed (Beale *et al* 1981, Bishop 1978a, b, Bruce 1980, Bruce and Schneider 1977, Bruce *et al* 1979, Schneider and Stoll 1980), which in dimensions $d = 1, 2$ are in fair agreement with the more fundamental dynamic diagnostics (general d). In particular, in $d = 1, 2$, renormalisation group (RG) methods have been suggested. These have ranged from approximate momentum space RG studies of distribution functions for block coordinates, to approximate real space

† Work performed under the auspices of the US DOE.

‡ There is also qualitative agreement with some experiments (see Bruce 1980); however, an additional lower crossover temperature is also characteristic (see Schneider and Stoll 1980), which can also be anticipated from the approximate criterion we suggest here (see text).

decimation RG approaches. In the latter case, a criterion based on *non-critical* RG *flow* was suggested (Beale *et al* 1981) for $T_x(\theta)$: namely, that $T_x(\theta)$ separates between flows to Ising and Gaussian (sometimes referred to as 'high-symmetry') high-T fixed points. It is important to emphasise that (i) the above results should apply generally to all models of the $\lambda\phi^4$ *class* (i.e. Hamiltonians with unbounded doubly degenerate local potentials), (ii) discontinuities are *not* expected at $T_x(\theta)$ in any thermodynamic (or dynamic) properties, and (iii) existing static criteria in $d>2$ are very indecisive.

In this Letter we present a model belonging to, and entirely representative of, the $\lambda\phi^4$ class whose thermodynamic properties we have been able to decompose *naturally* into Ising-like and Gaussian model contributions (all d). These subsystems are automatically characterised by domain-wall and (monotonic well) quasi-harmonic excitations respectively. We feel that a transparent example has been lacking in this general area. The present model will allow the investigation of criteria for $T_c(\theta)$ and for the quasi-crossover at $T_x(\theta)$ quite precisely. It will be a valuable test of various RG techniques and in addition allow a much clearer analysis of d-dependence. The model can be posed as a conventional spin model with double-Gaussian spin weight function. This spin model is of interest in its own right because of recent attempts to study its critical properties with high-T series (Rehr and Nickel 1981, Fisher 1981). In the lattice dynamics context we typically consider a bare Hamiltonian of the form (Bruce 1980, Beale *et al* 1981)

$$H\{X_i\} = \sum_{i=1} V(X_i) + \tfrac{1}{2}C\sum_{\{ij\}}(X_i - X_j)^2, \qquad (1)$$

where N is the number of lattice sites, the sum over $\{ij\}$ is over nearest-neighbour sites, and V is a (fixed) local potential with two degenerate minima characterised by well width, depth and location. For instance, the prototype $\lambda\phi^4$ model itself has

$$V(x) = -\tfrac{1}{2}Ax^2 + \tfrac{1}{4}Bx^4, \qquad (2)$$

where A and B are usually taken to be T-independent. Since various parametrisations have been adopted in the literature, we will first present our model and its decomposition in the general form of a spin model with spin weight distribution

$$\begin{aligned}\rho(x) &= \tfrac{1}{2}(2\pi w^2)^{-1/2}\{\exp[-(x-v)^2/2w^2] + \exp[-(x+v)^2/2w^2]\} \\ &= (2\pi w^2)^{-1/2}\exp(-v^2/2w^2)\exp(-x^2/2w^2)\cosh(xv/w^2).\end{aligned}$$

For simplicity (and the class (1)), we consider here nearest-neighbour isotropic spin-type coupling. (Extension to anisotropic, long-range, etc, interactions does not affect our decomposition.) We use the simple result $\cosh\alpha = \frac{1}{2}\sum_{\mu=\pm1} e^{\alpha\mu}$ to write the partition function Z following from (3) and

$$-\beta H = \sum_i \left(u\sum_{\{\delta\}} x_i x_{i+\delta} - t x_i^2\right), \qquad (4)$$

$$Z = [\tfrac{1}{2}(2\pi w^2)^{-1/2}\exp(-v^2/2w^2)]^N \sum_{\{\mu_i=\pm1\}} \int_{-\infty}^{\infty}\!\!\cdots\!\int \prod_{i=1}^{N} dx_i \times\exp\left[\sum_i\left(u\sum_{\{\delta\}} x_i x_{i+\delta} - t x_i^2 - \frac{x_i^2}{2w^2} + \frac{v}{w^2}x_i\mu_i + Hx_i\right)\right]. \qquad (5)$$

Here $\{\delta\}$ is (half) the nearest-neighbour set, u gives the spin coupling strength, the t-term is introduced for generality (cf (1)), and we have included a magnetic field term. Introducing Fourier transform variables ($\boldsymbol{q}$ restricted to the first Brillouin zone) (see e.g. Baker 1962)

$$z_{\boldsymbol{q}} = N^{-1/2} \sum_{\boldsymbol{j}} \exp(2\pi i \boldsymbol{q} \cdot \boldsymbol{j}) x_{\boldsymbol{j}}, \qquad \nu_{\boldsymbol{q}} = N^{-1/2} \sum_{\boldsymbol{j}} \exp(2\pi i \boldsymbol{q} \cdot \boldsymbol{j}) \mu_{\boldsymbol{j}}, \tag{6}$$

and re-expressing, we find after some algebra that all $z_{\boldsymbol{q}}$-dependence can be removed by integration with the final result

$$Z = [\tfrac{1}{2}\exp(-v^2/2w^2)]^N Z_G Z_I, \tag{7a}$$

$$Z_G = \exp\left\{\frac{\tfrac{1}{2}NH^2w^2}{1+2w^2(t-du)} - \tfrac{1}{2}\sum_{\boldsymbol{q}} \ln\left[1+2w^2\left(t-u\sum_{\tau=1}^{d}\cos 2\pi q_\tau\right)\right]\right\}, \tag{7b}$$

$$Z_I = \sum_{\{\mu_i=\pm1\}} \exp\left[\frac{v^2}{2w^2}\sum_{\boldsymbol{i},\boldsymbol{j}} \mu_{\boldsymbol{i}}\left(N^{-1}\sum_{\boldsymbol{q}} \frac{\exp[2\pi i \boldsymbol{q}\cdot(\boldsymbol{j}-\boldsymbol{i})]}{1+2w^2(t-u\sum_{\tau=1}^{d}\cos 2\pi q_\tau)}\right)\mu_{\boldsymbol{j}} + \frac{Hv}{1+2w^2(t-du)}\sum_{\boldsymbol{i}}\mu_{\boldsymbol{i}}\right]. \tag{7c}$$

In writing (7) we have specialised (for simplicity only) to the hypersimple cubic family. Equation (7) is our central result. For we see that (i) Z_G is simply the *Gaussian model* (Berlin and Kac 1952) partition function with magnetic field $\equiv Hw$ and reduced temperature $\beta J \equiv uw^2/(1+2w^2t)$, and (ii) Z_I is an *Ising model* (Domb 1974) partition function with the simple modification that $J(\boldsymbol{i}-\boldsymbol{j})$ (the $\mu_{\boldsymbol{i}}\mu_{\boldsymbol{j}}$ interaction coefficient) is long-ranged but decays *exponentially* with distance according to a familiar nearest-neighbour lattice Green function (see (7*c*)). Specifically, we can show that (7*c*) will arise from

$$J(\boldsymbol{i}-\boldsymbol{j}) \simeq (v^2/4w^2)(uw^2)^{-(d+1)/4}|\boldsymbol{i}-\boldsymbol{j}|^{-(d-1)/2}\exp[-|\boldsymbol{i}-\boldsymbol{j}|(uw^2)^{-1/4}] \tag{8}$$

(for later purposes we have specialised to $t=ud$). The decay is a pure exponential at all non-zero separations for $d=1$ and is a soluble model (Baker 1961). On the basis of (7) we can expect, in general, two critical points for fixed w: first a Gaussian critical point, T_G from $2dw^2u = 1+2w^2t$, and second an Ising-class transition at $T_c(w)$. We discuss $T_c(w)$ in more detail below, but remark here that $T_c(w) > T_G(w)$, for all w except in the limit $v \to 0$ where they coincide.

Considering (1), we see that, in effect, the spin weight distribution acquires a T-dependence, which has some interesting consequences. Our model corresponds to

$$\beta V(x) = \tfrac{1}{2}(x/w)^2 - \ln\cosh(xv/w^2), \tag{9}$$

which should be compared with (2). For illustration we consider the parametrisation

$$w = K^{-1/4}(1+\theta)^{-1/4}, \qquad u = K, \qquad v = (\theta/1+\theta)^{1/2}, \qquad t = dK. \tag{10}$$

Note that displacive and order–disorder limits now correspond to $\theta = 0$ and ∞, respectively.

Observe first that this parametrisation maps the previous Gaussian line of critical points to the line $K=\infty$. To examine the Ising critical points $K_c(\theta)$ we compute the total interaction strength per spin in Z_I, because experience has shown that the ferromagnetic Ising model critical point is determined by a critical value of the total strength, which value is only weakly dependent on lattice structure, etc (Domb 1974, Bricmont and Fontaine 1981). From the terms in (7*c*) and from (10) this result is easily found as $S = \tfrac{1}{2}\theta(K/1+\theta)^{1/2} - S_0$, where S_0 is a self-interaction term. From (7*c*) with $i = j$,

$$S_0 = \frac{\frac{1}{2}\theta(K/1+\theta)^{1/2}}{1+2d(K/1+\theta)^{1/2}} N^{-1} \sum_q \left(1 - \frac{2(K/1+\theta)^{1/2}}{1+2d(K/1+\theta)^{1/2}} \sum_{\tau=1}^{d} \cos 2\pi q \tau_d\right)^{-1}. \tag{11}$$

We have studied S_0 in detail. It does not alter S except for $d = 1$ where $S_0 = \frac{1}{2}S$ ($K \to \infty$) and in the Ising limit $\theta \to \infty$ (all d) where $S_0 = S$ to leading order in θ. In the last case we find a nearest-neighbour Ising model explicitly with $S_0 = S - dK + O(\theta^{-1/2})$, so that the Ising result for K_c is exactly recovered with deviation $\propto \theta^{-1/2}$ for large θ. For the Ising limit the critical strength S is a constant depending only on lattice and dimensionality: $S(d = 1) = \infty$; $S(\text{square}) = (1.13460)^{-1}$; $S(\text{cubic}) = (1.50360)^{-1}$; $S(\text{mean field}) = \frac{1}{2}$. As θ is varied, we expect the critical strength will vary only weakly in the Ising mean-field range, since the Ising interaction decays exponentially for large separations. Our conclusions are therefore

$d = 1$: $K_c(\theta) = \infty$, for all θ,

$d = 2$: $1 \leqslant \theta^2 K_c(\theta) \leqslant 3.11$, $\theta \to 0$, $K \to K_c(\text{Ising}) + O(\theta^{-1/2})$, $\theta \to \infty$, (12)

$d = 3$: $1 \leqslant \theta^2 K_c(\theta) \leqslant 1.77$, $\theta \to 0$, $K \to K_c(\text{Ising}) + O(\theta^{-1/2})$, $\theta \to \infty$.

We have indicated $K_c(\theta)$ in figure 1. The picture for $K_c(\theta)$ is qualitatively consistent with the RG results of Beale *et al* (1981), and the main differences arise from our choice of parametrisation.

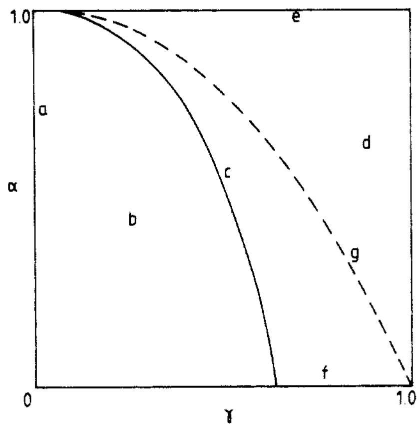

Figure 1. Features of the $\alpha = 1/(1+\theta)$, $\gamma = 1/(1+K)$ plane. (a) The $\gamma = 0$ line is a line of Gaussian critical points; (b) region is a modified low-temperature (two-phase) Ising region; (c) line of Ising-like critical points; (d) this whole region (including the point $\alpha = 0$, $\gamma = 1$) flows under the block-spin RG to the point $\alpha = 1$, $\gamma = 1$ for infinite block size; (e) pure Gaussian model on the line $\alpha = 1$; (f) pure Ising model on the line $\alpha = 0$; (g) the broken line indicates the line of equal strength Gaussian and Ising interactions.

Considering the suggested quasi-crossover from Gaussian to order–disorder fluctuations, we observe immediately from (7) that this general picture is also supported qualitatively. For small θ we see that the Gaussian contribution dominates the Ising one, except *very* near the critical line $K_c(\theta)$ where Ising behaviour (albeit with long-range interactions) necessarily dominates. By contrast, for large θ we see that the Gaussian contributions become very small and the Ising behaviour is dominant for all K except for large enough K^{-1}. The Ising regime can also be understood from the interaction range of the generalised Ising model in (7*c*). The Ising interactions, as expected, become short-ranged in the order–disorder limit $\theta \to \infty$, but increasingly long-ranged as the displaciveness increases (θ decreases). Critical exponents are Ising-like for all $\theta > 0$. For $\theta = 0$ the model passes continuously to a pure Gaussian form. (The point $\theta = 0 = K^{-1}$ requires special treatment.)

At this point it is appropriate to recall a general theorem (Baker and Krinsky 1977, Newman 1980) which does not appear to have been fully appreciated in this context.

Theorem. Any translationally invariant ferromagnetic Ising model (that is to say, every single-spin distribution is identical and has a finite variance, and the spin–spin interaction energy, $-J(i, j)$, between the spins at sites i and j is of the form $J(i-j) > 0$) at a temperature at which the magnetic susceptibility, χ, is finite has the property that the limit of the distribution of the block-spin variables $S_k = (\Sigma_{i=0}^{n-1} X_{nk+i})n^{-d/2}$ converges to independent Gaussian random variables of variance χ.

The consequence of this theorem is that for all $0 \leq \theta \leq \infty$ and $0 \leq K < K_c(\theta)$, the block-spin, RG fixed-point Hamiltonian for both $\lambda\phi^4$ models and the present double-Gaussian model, among others, is just the non-interacting Gaussian model. The theorem is in conflict with the results of Beale *et al* (1981) based on decimation RG instead of (real space) block-spin RG, which suggests flow to 'Ising high-T fixed points' for sufficiently order–disorder bare Hamiltonians. This contradiction of the theorem may be an artifact of decimation and/or their separation of first- and second-neighbour interactions under iteration. However, we emphasise that global flows rather than local flows are addressed by the above theorem.

Since there are no thermodynamic discontinuities associated with the suggested non-critical, displacive–order–disorder crossover at $K_x(\theta)$, an unambiguous criterion is difficult to define. The criterion based on RG flow (Beale *et al* 1981) is evidently a balance of *strengths* of competing local flow directions. In the same spirit we can compare the total interaction strengths per spin, S_G and S_I, in the cleanly divided Gaussian and Ising components of (7). With parametrisation (10), S_G is easily identified as $d(K/1+\theta)^{1/2}[1+2d(K/1+\theta)^{1/2}]^{-1}$, and from our earlier discussion $S_I \simeq \frac{1}{2}\theta K^{1/2}$ for small θ. Equating S_G with S_I suggests $K_x(\theta) = \theta^{-2} < K_c(\theta)$, and thus $K_c(\theta)/K_x(\theta) =$ constant ($d > 1$) in this limit. As for $K_c(\theta)$, there is again qualitative agreement with RG results; this agreement becomes very striking if a more closely analogous parametrisation to their model is chosen. Further work, which will be described in detail elsewhere, shows clearly the nature of the relationship of that RG criterion to the equal strength criterion. The natural decomposition (7) is being used to study competing contributions in a variety of thermodynamic properties. These may provide clearer diagnostics for $K_x(\theta)$ and show the weaker signals anticipated in $d > 2$, than in $d = 2$. Similarly, a critical analysis of RG techniques and of high-T series analysis can be given based on this separable model.

References

Baker G A Jr 1961 *Phys. Rev.* **122** 1477
—— 1962 *Phys. Rev.* **126** 2071

Baker G A Jr and Krinsky S 1977 *J. Math. Phys.* **18** 590
Beale P D 1981 *Phys. Rev.* B **24** 6711
Beale P D, Sarker S K and Krumhansl J A 1981 *Phys. Rev.* B **24** 266
Berlin T H and Kac M 1952 *Phys. Rev.* **86** 821
Bishop A R 1978a *Physica* **93A** 82
—— 1978b in *Lattice Dynamics* ed M Balkanski (Paris: Flammarion Sciences) pp 144 *et seq.*
Bricmont J and Fontaine J-R 1981 *45th Stat. Mech. meeting, Rutgers University*; and *preprint*
Bruce A D 1980 *Adv. Phys.* **29** 111
Bruce A D and Schneider T 1977 *Phys. Rev.* B **16** 3991
Bruce A D, Schneider T and Stoll E 1979 *Phys. Rev. Lett.* **43** 1284
Domb C 1974 in *Phase Transitions and Critical Phenomena* vol 3 ed C Domb and M S Green (New York: Academic) p 357
Fisher M E 1981 *private communication*
Newman C M 1980 *Commun. Math. Phys.* **74** 119
Rehr J J and Nickel B G 1981 *J. Stat. Phys.* **24** 710
Schneider T and Stoll E 1980 *Ferroelectrics* **24** 67; and private communications