Critical and crossover behavior in the double-Gaussian model on a lattice

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The double-Gaussian model, as recently introduced by Baker and Bishop, is studied in the context of a lattice-dynamics Hamiltonian belonging to the familiar ϕ^4 class. Advantage is taken of the partition-function factorability (into Ising and Gaussian components) to place bounds on the Ising-class critical temperature for various lattice dimensions and all degrees of displaciveness in the bare Hamiltonian. Further, a simple criterion for a noncritical and nonuniversal crossover from order-disorder to Gaussian behavior is evaluated in numerical detail. In one and two dimensions these critical and crossover properties are compared with predictions based on real-space decimation renormalization-group flows, as previously exploited in the ϕ^4 model by Beale *et al.* The double-Gaussian model again introduces some unique analytical advantages.

I. INTRODUCTION

Structural phase transitions usually have the distinguishing feature that the order parameter derives from microscopic degrees of freedom which can take on continuous values (e.g., latticeion displacements), in contrast to spin systems. If one is unconcerned with any physics except the critical behavior, then it is now well understood¹ that microscopic details are in a sense secondary to the universality class which dominates the critical behavior. In fact, however, both real and computer experiments examine properties of systems both at and away from critical regions, and significant qualitative changes are observed over the wider regime. It is this broader perspective which has motivated this and our related prior work.²⁻⁴ In particular, we have previously found significant qualitative (but noncritical) changes in the statistical-mechanical character of the system, removed from any critical behavior, which is well determined by application of decimation renormalization-group (RG) methods in lattice space and examination of the resulting flow maps. $^{2-3}$

Previously [Beale, Sarker, and Krumhansl^{2,3} (BSK)] these questions were studied in the context of the ϕ^4 model which is described in the static

limit by the lattice Hamiltonian

$$H\{x_{\vec{i}}\} = \sum_{\vec{i}=1}^{N} V(x_{\vec{i}}) + \frac{1}{2}C \sum_{\{\vec{i},\vec{j}\}} (x_{\vec{j}} - x_{\vec{i}})^{2},$$
(1.12)

$$V(x)(\phi^4) = -\frac{1}{2}Ax^2 + \frac{1}{4}Bx^4 , \qquad (1.1b)$$

where $\{x_{\vec{i}}\}$ are displacive coordinates, N is the number of lattice sites, the sum over $\{\vec{i}, \vec{j}\}$ is over nearest-neighbor pairs, and the main feature of the local potential V is that it possesses two degenerate minima. A, B, and C are positive constants. Recently, though, the very useful observation has been made [Baker and Bishop⁴ (BB)] that another double-well model, the double-Gaussian weighting of a spin system, is equivalent to a local potential V in (1.1a) of the form

$$\beta V(x) = \frac{1}{2} \left(\frac{x}{w} \right)^2 - \ln \cosh \left(\frac{xv}{w^2} \right). \quad (1.1c)$$

Here $\beta = (k_B T)^{-1}$. The parameters v and w will be discussed in Secs. II and III. For v > w, V in (1.1c) preserves a degenerate double-well structure. In the context of lattice dynamics it has become customary to refer to "displacive" and "order-disorder" limits in the bare Hamiltonian (1.1a). These correspond, respectively, to shallow- and

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deep-well limits in V compared to the strain energy; then x variations from site-to-site are, respectively, small or large compared to a lattice spacing. In (1.1b) for example, the limits are, respectively, C >> A and C << A. The choice (1.1c) leads to a factorizable partition function—it can be expressed exactly as the product of Ising- and Gaussianmodel partition functions. This notable fact directly proves Ising-class universal critical properties. It also allows us to reexamine many questions we studied numerically only for the ϕ^4 model,^{2,3} and that is the purpose of the study we present here.

We find again the same important characteristic features (but noncritical and nonuniversal) which were found for the ϕ^4 model. Near the critical line a double-well system, which will undergo a structural phase transition, falls into the Ising universality class. However, away from the critical line (far away in 1D, less in 2D, and very near in 3D and higher dimensions) there is, in addition, a clear crossover from Ising behavior to an anharmonic Gaussian behavior. [The crossover occurs closer to T_c as the displaciveness of the bare Hamiltonian increases but, on universality grounds, the critical behavior will ultimately always be "order-disorder" ("Ising") in character.] This is seen now both from flow maps in decimation RG and by determining the crossover from Ising to Gaussian domination in the factorized partition function of the double-Gaussian model. Although not expressed quantitatively for a specific dynamical quantity,⁵ we believe² that this crossover signals a change from significant short-range order in the form of clusters (domains) to more random fluctuations of a collection of highly anharmonic (effective) oscillators.

Our RG procedure leads only to a quantitative statement about the single-site-displacement probability-distribution function, which as Bruce has pointed out^{1,6} (in the present context) is not sufficient to determine critical behavior. This limitation must be emphasized. To truly examine ordering structures in the critical region it is necessarv to study variables which embrace many sites: the block-spin variable is such a quantity.^{6,7} For $T \neq T_c$, independent of displaciveness, the distribution of the block-spin variable tends to independent Gaussians^{4,7} in the limit of the block size going to infinity. For $T > T_c$ these Gaussians have zero mean and for $T < T_c$ the mean is proportional to the magnetization. Recently Bruce⁶ and Binder⁸ have established the nature of the block-spin probability-distribution function (pdf) at T_c for the

double-well potential and determined its universal features. In dimension 1D the block pdf consists of two δ -function peaks at $\pm x_0$ [well bottoms in (1.1)]; in 2D the pdf is smeared but still double peaked; but for 3D it is probably only singly peaked (and indeed purely Gaussian for d > 4), although an Ising-class phase transition is clearly occurring.

Our results below are consistent with the above picture, as follows: For both 1D ($T_c = 0$) and 2D ($T_c = T_{Ising}$) we find a double-peaked *single-site* pdf, not only near T_c , but in fact, for a significant region $T_c < T < T_x$, where T_x is the crossover temperature. We reemphasize that in general, our crossover condition is not expected to be universal. From preliminary studies for d > 2, we conclude that T_x is increasingly near to T_c as one would expect from Bruce's⁶ and Binder's⁸ results.

The organization of the remainder of the paper is as follows: In Sec. II we review the reduction⁴ of the partition function for a double-Gaussian potential to a Gaussian and an Ising factor. In Sec. III we first parametrize the double Gaussian to have the same limiting form as we used in the ϕ^4 model; the two important parameters are the well depth and either the position of the minima or the curvature there. We then discuss critical and crossover conditions for the double-Gaussian model; in particular, we obtain limiting behaviors analytically for the displacive (shallow-well) and order-disorder (deep-well) limits. The crossover region is discussed in the context of equal total interaction strengths⁴ in the partition function. In Sec. IV we carry out the decimation RG.^{2,3} Delightfully, in 1D this procedure can be carried through analytically for the double-Gaussian model; in 2D the procedure⁹ of Wilson and of Casher and Schwartz was used. The RG flow patterns are presented. We are left with one puzzle: In 1D the equal-strength criterion in Sec. III gives a dependence of the crossover line on temperature in the displacive limit which does not agree with the decimation RG result. The latter, however, is justifiable on physical grounds in terms of the density of domain boundaries and has been found by a number of authors.^{1,10} We suspect this disagreement to be an artifact, but as yet have not been able to explain it. However, for 2D both approaches predict the same form of logarithmic dependence in the displacive limit, and for d > 2the equal-strength criterion yields very plausible results for both the crossover and critical temperatures.

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II. SEPARATION OF THE PARTITION FUNCTION

In this section we give the main details of the partition-function decomposition reported by BB^4 for the double-Gaussian model. For generality we present the derivation in the form of a conventional continuous-spin model with spin-weight distribution

$$\rho(x) = \frac{1}{2} (2\pi w^2)^{-1/2} \left[\exp\left[-\frac{(x-v)^2}{2w^2} \right] + \exp\left[-\frac{(x+v)^2}{2w^2} \right] \right]$$
$$= (2\pi w^2)^{-1/2} \exp\left(-\frac{1}{2} v^2 / w^2 \right) \exp\left(-\frac{1}{2} x^2 / w^2 \right) \cosh(xv / w^2) .$$
(2.1)

Note that $\rho(x)$ approaches a pure (double δ function) Ising distribution as the parameter $w \rightarrow 0$ and a pure (single peaked) Gaussian one as $v \rightarrow 0$. Applications in the spin context are, in fact, of interest in their own right in view of recent high-temperature series analyses,¹¹ which attempt to clarify critical properties. We will not comment on those further here except to note (i) that the decomposition we show below should be a useful check on series results, and (ii) the decomposition holds generally for arbitrary spin couplings, including anisotropic and/or long-range interactions, etc. For the purpose of the application described in Sec. I, we will present the derivation here for the case of nearest-neighbor, isotropic spin coupling. The partition function is

$$Z = (2\pi w^2)^{-N/2} \exp\left(-\frac{1}{2}Nv^2/w^2\right) \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \prod_{\vec{i}} dx_{\vec{i}} \exp\left[\sum_{\vec{i}} \left[u\sum_{\{\vec{\delta}\}} x_{\vec{i}} x_{\vec{i}} + \vec{\delta} - tx_{\vec{i}}^2 - \frac{1}{2}\frac{x_{\vec{i}}^2}{w^2}\right]\right] \times \prod_{\vec{i}} \left[\cosh\left[\frac{vx_{\vec{i}}}{w^2}\right] \exp(Hx_{\vec{i}})\right].$$
(2.2)

Here N is the number of lattice sites, $\{\vec{\delta}\}$ is half the set of nearest neighbors, and we have included a magnetic field (H) term for generality.

The basis of our separation, as for the familiar pure Ising limit $w \rightarrow 0$, is to use the simple identity

$$2\cosh\alpha = \sum_{\mu=\pm 1} e^{\alpha\mu} , \qquad (2.3)$$

which in (2.2) yields

$$Z = \left\{ \frac{1}{2} (2\pi w^2)^{-1/2} \exp\left[-\frac{1}{2} (v/w)^2\right] \right\}^N$$

$$\times \sum_{\{\mu \overrightarrow{i} = \pm 1\}} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \prod_{\overrightarrow{i}} dx \overrightarrow{i} \exp\left\{ \sum_{\overrightarrow{i}} \left[u \sum_{\{\overrightarrow{\delta}\}} x \overrightarrow{i} x \overrightarrow{i}_{+} \overrightarrow{\delta} - \left[t + \frac{1}{2w^2} \right] x^2 \overrightarrow{i}_{+} + \left[\frac{v}{w^2} \right] x \overrightarrow{i} \mu \overrightarrow{i}_{+} + Hx \overrightarrow{i}_{-} \right] \right\}.$$

$$(2.4)$$

We now introduce Fourier transform variables,

$$z_{\vec{q}} = N^{-1/2} \sum_{\vec{j}} e^{2\pi i \vec{q} \cdot \vec{j}} x_{\vec{j}} ,$$

$$v_{\vec{q}} = N^{-1/2} \sum_{\vec{j}} e^{2\pi i \vec{q} \cdot \vec{j}} \mu_{\vec{j}} ,$$
(2.5)

with \vec{q} restricted to the first Brillouin zone of the reciprocal lattice. It follows from (2.5) that

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$$\sum_{\vec{i}} \sum_{\{\vec{\delta}\}} x_{\vec{i}} x_{\vec{i}+\vec{\delta}} = \sum_{\{\vec{\delta}\}} \sum_{\vec{q}} e^{-2\pi i \vec{q} \cdot \vec{\delta}} z_{\vec{q}} z_{-\vec{q}}$$
(2.6a)

$$= \sum_{\vec{q}} \left[\sum_{\tau=1}^{d} \cos(2\pi q_{\tau}) \right] z_{\vec{q}} z_{-\vec{q}} .$$
(2.6b)

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In (2.6b) we have specialized, for simplicity, to a hyper-simple-cubic-lattice of arbitrary dimension d. Equation (2.4) reduces to (it is straightforward to show that this is a canonical transformation) the following:

$$Z = \left[\frac{1}{2}(2\pi w^{2})^{-1/2} \exp\left(-\frac{1}{2}v^{2}/w^{2}\right)\right]^{N} \times \sum_{\{\mu_{\tau}^{-}=\pm1\}} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \prod_{\vec{q}} dz_{\vec{q}} \exp\left[-\sum_{\vec{q}} \left[-u\left[\sum_{\tau=1}^{d} \cos 2\pi q_{\tau}\right] + \frac{1}{2}w^{-2} + t\right] \left|z_{\vec{q}} + \frac{\frac{1}{2}\frac{v^{2}}{w^{2}}v_{-\vec{q}} + \frac{1}{2}N^{1/2}H\delta_{\vec{q},0}}{\frac{1}{2}w^{-2} + t - u\sum_{\tau=1}^{d} \cos 2\pi q_{\tau}}\right|^{2} + \frac{\frac{1}{4}\left|\frac{v}{w^{2}}v_{-\vec{q}} + N^{1/2}H\delta_{\vec{q},0}\right|^{2}}{\frac{1}{2}w^{-2} + t - u\left[\sum_{\tau=1}^{d} \cos 2\pi q_{\tau}\right]}\right].$$

$$(2.7)$$

Integrating over $z_{\vec{a}}$ and reexpanding $v_{-\vec{a}}$ in terms of $\{\mu_{\vec{i}}\}$, we find from (2.7) the central result

$$Z = \{\frac{1}{2} \exp[-\frac{1}{2}(v/w)^2]\}^N Z_G Z_I , \qquad (2.8a)$$

where

$$Z_{G} = \exp\left\{\frac{\frac{1}{2}NH^{2}w^{2}}{1+2w^{2}(t-du)} - \frac{1}{2}\sum_{\vec{q}}\ln\left[1+2w^{2}\left[t-u\sum_{\tau=1}^{d}\cos 2\pi q_{\tau}\right]\right]\right\},$$
(2.8b)

$$Z_{I} = \sum_{\{\mu_{\vec{i}}=\pm1\}} \exp\left[\frac{1}{2} \frac{v^{2}}{w^{2}} \sum_{\vec{i},\vec{j}} \mu_{\vec{i}} \mu_{\vec{j}}\right] N^{-1} \sum_{\vec{q}} \frac{\exp[2\pi i \vec{q} \cdot (\vec{j} - \vec{i})]}{1 + 2w^{2} \left[t - u \sum_{\tau=1}^{d} \cos 2\pi q_{\tau}\right]} + \frac{Hv \sum_{i} \mu_{\vec{i}}}{1 + 2w^{2} (t - du)}\right]. \quad (2.8c)$$

We see in (2.8) that the double-Gaussian partition function has been factored into (i) the partition function Z_G of a conventional Gaussian model^{12,13} with magnetic field Hw and reduced temperature $\beta J \equiv uw^2(1 + 2w^2t)^{-1}$, and (ii) the partition function Z_I of an Ising model with spin interaction range depending on w. Specifically, the $\mu \overrightarrow{} \mu \overrightarrow{}$ interaction coefficient, $J(\vec{i} - \vec{j})$, is generally long ranged but decays exponentially at large distances according to a familiar nearest-neighbor lattice Green's function. It is not hard to show that this Green's function [see (2.8c)] arises from

$$J(|\vec{i} - \vec{j}|) \sim \left(\frac{1}{2} \frac{v}{w}\right)^{2} (uw^{2})^{-(d+1)/4} \\ \times |\vec{i} - \vec{j}|^{-(d-1)/2} \\ \times \exp[-|\vec{i} - \vec{j}| (uw^{2})^{-1/2}]. \quad (2.9)$$

Results (2.9) are valid in all d > 1 for separations much larger than a lattice spacing; in 1D (an exactly soluble model¹³) the decay is a pure exponential at all nonzero separations. In writing (2.9) we have also specialized to t = ud for use in the application described in Sec. I (see Sec. III). It should be clear that the separation in (2.8) extends, with simple modifications, to many other thermodynamic quantities.

On the basis of (2.8) we deduce that there will, in general, be two critical points for fixed w: A Gaussian critical point, $T_G(w)$, determined from $2dw^2u = 1 + 2w^2t$, and an Ising-class critical point, $T_c(w)$. We estimate $T_c(w)$ in Sec. III. Here it is appropriate only to note that the method used in Sec. III leads to the general conclusion $T_c(w)$ $> T_G(w)$ for all w except the Gaussian limit v=0, where $T_c = T_G$. For the application described in

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Sec. I the Gaussian critical temperature is precisely $T_c \equiv 0$ in view of the parametrization (3.3), and therefore is not germane to this study. The Ising critical behavior is in this way established for all v, w of physical interest and applies whether the initial distribution $\rho(x)$ is singly $(v \le w)$ or doubly (v > w) peaked. In the limit $w \to \infty$, the Ising interaction range diverges and mean-field theory is expected to apply, a fact which we use in Sec. III. The actual forms of $T_c(w)$ and $T_G(w)$ depend sensitively on the particular application, so we now turn to the specific case which we wish to analyze here.

III. ϕ^4 PARAMETRIZATION: CRITICAL AND CROSSOVER LINES

In the context of the lattice Hamiltonian (1.1) we see that our double-Gaussian model (2.1) corresponds to a local potential [see (1.1c)]

$$\beta V(x) = \frac{1}{2} \left[\frac{x}{w} \right]^2 - \ln \cosh \left[\frac{xv}{w^2} \right].$$
(3.1)

The temperature dependence introduced in (3.1) has some specific consequences with regard to the form of T_G and T_c (below) and deductions also depend very sensitively on the choice of v and w in (3.1). To be precise, we wish to compare as closely as possible with the ϕ^4 model, as parametrized in Refs. 2 and 3, viz. local potential

$$\beta V(x) = -\frac{1}{2} K \Theta x^2 + \frac{1}{4} K (1 + \Theta) x^4 , \qquad (3.2)$$

 $(v/w)^2 \longrightarrow 1 + (\frac{1}{3}K)^{1/2} \Theta$ as $\Theta \rightarrow 0$,

 $v \longrightarrow \left[\frac{\Theta}{1+\Theta}\right]^{1/2} \text{ as } \Theta \to \infty ,$

 $v \longrightarrow (3K)^{-1/4} + \frac{2}{15}(3K)^{1/4}\Theta$ as $\Theta \to 0$,

 $w \longrightarrow (3K)^{-1/4} - \frac{1}{30} (3K)^{1/4} \Theta \text{ as } \Theta \rightarrow 0$,

where

$$\beta^{-1} = k_B T = B^{-1} C^2 (1 + \Theta) K^{-1},$$

 $\Theta = A / C.$

This parametrization preserves a double-well structure for all $T < \infty$ and $\Theta > 0$: $\Theta = 0$ corresponds to the displacive limit and $\Theta = \infty$ the pure Ising limit. To reproduce this feature in (3.1), there are several possibilities for v and w. The most conventional choices are to match the ϕ^4 -well minima location ($x = \pm [\Theta/(1+\Theta)]^{1/2}$) and depth ($\frac{1}{4}[K\Theta^2/(1+\Theta)]$) [(3.3a) and (3.3b)], or local curvature at the minima (2K Θ) (3.3c). Comparing with (3.1) we find that these features lead, respectively, to the conditions

$$\left(\frac{\Theta}{1+\Theta}\right)^{1/2} = v \tanh\left[\frac{v}{w^2}\left(\frac{\Theta}{1+\Theta}\right)^{1/2}\right], \quad (3.3a)$$

$$v^{2} = \frac{\Theta}{1+\Theta} \left\{ 1 - \exp\left[-\frac{\Theta}{1+\Theta} \left[w^{-2} + \frac{1}{2} K \Theta \right] \right]^{-1} \right\}$$
(3.3b)

$$v^2 = w^2 - 2K\Theta w^4 + \frac{\Theta}{1+\Theta} . \qquad (3.3c)$$

We note in passing that the necessary and sufficient condition for (3.1) to have a double-well structure is v > w.

In general, we have solved (3.3a) and (3.3b) or (3.3c) for v and w numerically. However, it is instructive to determine several limiting behaviors analytically. This requires careful and consistent expansion of Eqs. (3.3). The relevant results are as follows:

(3.4a)

(3.4b)

$$w \longrightarrow (K\Theta/2)^{-1/2} \text{ as } \Theta \rightarrow \infty$$
, (3.4e)

$$(v/w)^2 \longrightarrow 1 + (\frac{1}{3}K)^{1/2} \Theta(1+\Theta)^{-1/2}$$
 as $K \to 0$, (3.4f)

$$v \longrightarrow [3K(1+\Theta)]^{-1/4} [1 + \frac{1}{2}(\frac{1}{3}K)^{1/2}\Theta(1+\Theta)^{-1/2}] \text{ as } K \to 0, \qquad (3.4g)$$

$$w \longrightarrow [3K(1+\Theta)]^{-1/4}[1+O(\Theta^2)] \text{ as } K \to 0.$$
 (3.4h)

The results (3.4) are given for the case (3.3a) solved with (3.3b) (which will also be used in Sec. IV). If (3.3c) is used instead of (3.3b), there are changes in some coefficients but not powers of Θ or K. To complete the mapping of our general double-Gaussian model (2.1) onto the ϕ^4 model [(1.1) and (3.2)], we identify

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 $u = K, \quad t = dK \quad , \tag{3.5}$

so that the partition function becomes

$$Z = \{\frac{1}{2} \exp[-\frac{1}{2} (v/w)^2]\}^N Z_G Z_I , \qquad (3.6a)$$

$$Z_{G} = \exp\left\{\frac{1}{2}NH^{2}w^{2} - \frac{1}{2}\sum_{\vec{q}}\ln\left[1 + 2Kw^{2}\left[d - \sum_{\tau=1}^{d}\cos(2\pi q_{\tau})\right]\right]\right\},$$
(3.6b)

$$Z_{I} = \sum_{\{\mu_{\vec{i}}=\pm1\}} \exp\left[\frac{1}{2}\left[\frac{v}{w}\right]^{2} \sum_{\vec{i},\vec{j}} \mu_{\vec{i}} \mu_{\vec{j}}\right] \left[N^{-1} \sum_{\vec{q}} \frac{\exp[2\pi i \vec{q} \cdot (\vec{j}-\vec{i})]}{1+2Kw^{2}\left[d-\sum_{\tau=1}^{d} \cos 2\pi q_{\tau}\right]}\right] + Hv \sum_{\vec{i}} \mu_{\vec{i}}\right].$$
 (3.6c)

We remark that the restriction t = du, Eq. (3.5), is relevant to the lattice model (1.1) which we are considering, but is of course not necessary in general. If, however, t < du then the range of w's in (2.1) for which the model (2.2) is defined is restricted,¹⁴ and if t > du, then the Gaussian critical point is not as simple as we find below.

We are now in a position to discuss the interaction strengths per spin^{4,15} for the separated Ising and Gaussian components (3.6b) and (3.6c). These will be denoted S_I and S_G , respectively. $S_I(\Theta, K)$ will take a critical value¹⁵ at the Ising critical line $K_c(\Theta)$, and comparing S_G and S_I is one plausible criterion for a non-critical Ising-Gaussian crossover, which we wish to evaluate quantitatively (other criteria are being studied). The Gaussian strength S_G is well known.^{12,13,15} In the notation of (3.6b) this is

$$S_G = dKw^2 (1 + 2dKw^2)^{-1} . (3.7)$$

Evaluation of S_I requires careful evaluation and subtraction of the self-interaction term. From (3.6c) we find

$$S_{I} = \frac{1}{2} \left[\frac{v}{w} \right]^{2} \left[1 - f_{d} (2Kw^{2}) \right], \qquad (3.8a)$$

$$f_d(\alpha) = N^{-1} \sum_{\vec{q}} \left[1 + \alpha \left[d - \sum_{\tau=1}^d \cos(2\pi q_\tau) \right] \right]^{-1}$$
(3.8b)

$$= (2\pi)^{-d} \int_{-\pi}^{\pi} dq_1 \cdots \int_{-\pi}^{\pi} dq_d \left[1 + \alpha \left[d - \sum_{\tau=1}^{d} \cos q_\tau \right] \right]^{-1}$$
(3.8c)

$$= \alpha^{-1} \int_0^\infty dy \, e^{-y/\alpha} [e^{-y} I_0(y)]^d \,, \tag{3.8d}$$

with I_0 the modified Bessel function of zero order.

The parametrization (3.3) maps the line of Gaussian critical points discussed in Sec. II to the line $K = \infty$ (T=0). The Ising critical line remains at positive T except for $\Theta = 0$. Experience has shown¹⁵ that the ferromagnetic Ising-model critical point $K_c(\Theta)$ is determined by a critical value of the total strength S_I^c , the value of which is only weakly dependent on lattice structure, range of interaction, etc. In the Ising limit $w \rightarrow 0, \Theta \rightarrow \infty$,

 $S_1^c(\text{square}) = 0.88137 \text{ and } S_1^c(\text{cubic}) = 0.66507.$ In the opposite limit $\Theta \rightarrow 0, K \rightarrow \infty$, the Ising component interaction range becomes infinite [cf. (2.9) and (3.3)], and the mean-field critical strength¹⁵ should apply there (all d): $S_1^c(\text{mean field}) = \frac{1}{2}$. In $d=1, S_I^c = \infty$ so that $K_c = \infty$. These various critical strengths will bound $S_I^c(\Theta)$ for arbitrary Θ , since the Ising interaction in our model decays exponentially with distance for large separations. Based on this reasoning, it is possible to calculate upper and lower bounds on the critical coupling $K_c(\Theta)$. The upper bound $K_c^U(\Theta)$ is given by

$$S_I^c(\text{Ising limit}) = \frac{1}{2} \left[\frac{v}{w} \right]^2 \left[1 - f_d(2K_c^U w^2) \right],$$
(3.9)

where v and w are determined from Eqs. (3.3) as before. The lower bound $K_c^L(\Theta)$ is given by

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$$S_{I}^{c}(\text{mean field}) = \frac{1}{2}$$
$$= \frac{1}{2} \left(\frac{v}{w} \right)^{2} \left[1 - f_{d}(2K_{c}^{L}w^{2}) \right]. \quad (3.10)$$

The two curves $K_c^U(\Theta)$ and $K_c^L(\Theta)$ are shown in Fig. 1 for 2D along with three critical couplings $K_c(\Theta)$ determined from molecular-dynamics simulations on the ϕ^4 model.⁵ Note that these points lie between the upper and lower bounds as expected. (Results for the double-Gaussian model will be very similar to those for ϕ^4 with the parametrization adopted here, and identically so in the Ising limit.¹⁶)

It is possible to calculate $K_c(\Theta)$ exactly in the Ising and displacive limits based on one plausible assumption: that the critical value of the total strength S_I^c is slowly varying near the two limits. Considering first the Ising limit $(\Theta \rightarrow \infty, Kw^2 \rightarrow 0)$ we find that equation (3.8d) expands as

$$f_d(\alpha) \simeq 1 - d\alpha + d(d + \frac{1}{2})\alpha^2 . \qquad (3.11)$$

If $S_I^c = S_I^c$ (Ising limit) + $O(\alpha^2)$, then we find the following with the use of Eqs. (3.4d) and (3.4e):

$$S_{I}^{c} = \frac{1}{2} \left[\frac{v}{w} \right]^{2} \left[2Kw^{2} - 4K^{2}w^{4}d(d + \frac{1}{2}) \right] \quad (3.12a)$$
$$= dK_{c} \left[1 - \frac{4d + 3}{\Theta} + O(\Theta^{-2}) \right], \quad (3.12b)$$

which finally leads to

$$K_{c}(\Theta) \simeq K_{c}(\infty) \left[1 + \frac{4d+3}{\Theta} \right],$$
 (3.13)

for $\Theta \gg 1$ and where $K_c(\infty) = 0.4407$ in 2D and 0.2217 in 3D. We see that the well-known¹⁵ nearest-neighbor Ising critical temperature is correctly reproduced. Furthermore, the order of corrections (Θ^{-1}) as Θ decreases from ∞ are consistent with alternative calculations.^{2,17} In addition, in this "strong-coupling" regime our result (3.6c) agrees with previous findings¹⁷ in ϕ^4 models that in that regime the Ising and Gaussian components separate and that the interaction range of the relevant Ising model increases as Θ decreases from ∞ .

Near the displacive limit ($\Theta \ll 1$) the Ising interaction is very long ranged near criticality [see Eq. (2.9)], so we expect $S_I^c \rightarrow S_I^c$ (mean field). Assuming¹⁸ this we find

$$\frac{1}{2} = \frac{1}{2} \left(\frac{v}{w} \right)^2 \left[1 - f_d(2Kw^2) \right].$$
(3.14)



FIG. 1. Critical temperature $K_c(\Theta)$ as a function of the displaciveness Θ for the double-Gaussian model in two dimensions: $K_c^U(---)$ and $K_c^L(\cdots)$ are upper and lower bounds to K_c [see Sec. III. As described there, we expect that $K_c(\Theta)$ asymptotically approaches K_c^L as $\Theta \rightarrow 0$ and K_c^U as $\Theta \rightarrow \infty$]; $K_c(\Theta)$ deduced from decimation RG methods for the ϕ^4 model (Burkhardt and Kinzel, Ref. 15) is shown for comparison (—), together with available molecular-dynamics data (\blacktriangle).

Then with the use of Eqs. (3.3a)-(3.3c) [whose use is justified by the final forms (3.17) and (3.19) below] we get

$$(\frac{1}{3}K_c)^{1/2}\Theta \simeq f_d(2(\frac{1}{3}K_c)^{1/2})$$
 (3.15)

Now we need an asymptotic expansion of $f_d(\alpha)$ for large α ($\Theta \rightarrow 0, K \rightarrow \infty$: $K_c \rightarrow \infty$ as $\Theta \rightarrow 0$, see below). For 1D, $f_1(\alpha) = (1+2\alpha)^{-1/2}$. For d > 2,

$$f_{d}(\alpha) = 2\alpha^{-1}a(d) + O(\alpha^{-2}),$$

$$a(d) = \frac{1}{2} \int_{0}^{\infty} dy [e^{-y}I_{0}(y)]^{d}.$$
(3.16)

Equation (3.16) implies in (3.15)

$$K_c \Theta \simeq 3a(d), \quad \Theta \ll 1, \quad d > 2$$
 (3.17)

where numerical estimates give a(3)=0.2527, a(4)=0.1549, a(6)=0.0931, etc. The form (3.17) agrees with well-established results¹ for d > 2.

For two dimensions we find¹⁸ (combining

asymptotic and numerical estimates) the following:

$$f_2(\alpha) = (2\pi\alpha)^{-1}(\ln\alpha + C) + O(\alpha^{-2})$$
, (3.18)

where $C \simeq 2.77259$. The critical line is then given by

$$\frac{8\pi}{3}K_c\Theta \simeq \ln K_c + 5.832\,86\;. \tag{3.19}$$

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For sufficiently small Θ , the critical line has the logarithmic correction displayed by Eq. (3.19). However, note that the logarithmic term is not important until $\ln K_c \geq 6$, i.e., for $\Theta \leq 0.0035$, $K_c \geq 400$. This is a very low temperature and so the logarithmic correction might be quite difficult to distinguish in a molecular-dynamics simulation: Thus far, such small values have not been investigated. The logarithmic behavior has been predicted before^{18,19} but the sizable constant term in Eq. (3.19b) has not previously been noticed. The approximate RG scheme used in Sec. IV also correctly predicts the logarithmic behavior, but not the value of the constant term in (3.19b) or the coefficient of $K_c \Theta$.

We now leave the discussion of critical behavior and turn to the notion of an Ising-Gaussian noncritical crossover. As discussed in Sec. I, we emphasize that a strict or universal criterion is hard to imagine. However, the criterion determined from lattice decimation RG flow^{2,3} (Sec. IV) is evidently a strength criterion and it seems sensible as a first approach⁴ to compare this with the $S_G = S_I$ line, $K_x(\Theta)$. For $\Theta \rightarrow 0$, $K_x \rightarrow \infty$, the situation is quite similar to the previous discussion of $K_c(\Theta)$, except that we need the expansion of S_G . The use of (3.4c) in (3.7) gives

$$S_G = \frac{1}{2} \left[1 - \frac{1}{2d} \left[\frac{1}{3} K \right]^{-1/2} \right], \quad \Theta \to 0, \quad K \to \infty.$$
(3.20)

Equating (3.20) with S_I [Eq. (3.8)] gives

$$K_{x}\Theta = 3a(d) - \frac{3}{2d}, d > 2, \Theta \to 0$$
 (3.21a)

$$\frac{8\pi}{3}K_x\Theta = \ln K_x, \quad d = 2, \quad \Theta \to 0 \;. \tag{3.21b}$$

Equations (3.21a) and (3.21b) should be compared with (3.17) and (3.19). Notice that $K_x < K_c$ and $K_c/K_x \rightarrow 1+2da(d) \rightarrow 2$ as $d \rightarrow \infty$.²⁰ For 1D, $f_1(\alpha)$ can be evaluated exactly as

$$f_1(\alpha) = (1+2\alpha)^{-1/2}$$
. (3.22)

Equating (3.20) and (3.8b) with the use of (3.22) we obtain

$$K_x \Theta^{4/3} = 3(2)^{-4/3}, \ d = 1, \ \Theta \to 0$$
. (3.23)

The result for $K_x(d=1)$ is surprising and possibly disturbing since it differs from scaling arguments^{1,2,10} for $K_x(d=1,\Theta\rightarrow 0)$ based on the singleparticle probability-distribution function or the d=1 kink energy E_K : From (3.1) and (3.4) we find easily that $E_K \propto \Theta^{3/2}$, as $\Theta \rightarrow 0$ (displacive limit), in agreement with universal results for this class of potentials and the RG results deduced in Sec. IV. This discrepancy is as yet unresolved and may indicate a qualitative difference between "equal interaction strength" and other criteria; however, we are studying the partition function for the 1D double-Gaussian model to see if any $K\Theta^{3/2}$ behavior can be identified.

The high-temperature $(K_x \rightarrow 0)$ limit of the equal-strength line is also interesting and must be handled with care. From the use of (3.4d) and (3.4e) in (3.7) and (3.8), we might conclude that $K_x \Theta \rightarrow \frac{1}{2}$ as $\Theta \rightarrow \infty$. However, this line is evidently outside the range of validity of (3.4e) (except at the point $K=0, \Theta=\infty$; see below). In fact, we must consider the behaviors of v and w for $K\rightarrow 0$ but arbitrary Θ , i.e., results (3.4f)-(3.4h). These give

$$S_I \rightarrow \frac{1}{2} \left[\frac{v}{w} \right]^2 (2dKw^2) [1 - (1 + 2d)Kw^2 + \cdots],$$

(3.24a)

$$S_G \rightarrow dKw^2(1-2dKw^2+\cdots), \qquad (3.24b)$$

which, equating and using (3.4f) and (3.4h), yields (for all d)

$$K_x = 0$$
, all Θ (3.25a)

or

$$\Theta = 1 \text{ as } K_x \to 0$$
. (3.25b)

The equal-strength crossover line, therefore, flows from $\Theta = 0$ to a finite value (unity here for all d) as T changes from 0 to ∞ . This is in qualitative accord with the decimation RG results described in the following section and elsewhere.² However, in view of the differences expected between decimation and block RG flows (see Secs I and V), it is interesting to see from Eqs. (3.25a) and (3.25b) that $\Theta = 1, K_x = 0$ is actually a *bifurcation* point for equal-strength lines and that flow is quite undetermined at infinite temperature. [The location $\Theta = 1$ of the bifurcation point is independent of whether (3.3a) is solved with (3.3b) or (3.3c).] This undeterminedness partly reconciles the known⁷ blockspin-high-T fixed-point location $(T = \infty)$ with decimation flow.

Figure 1 compares the results concluded in this section for $K_c(\Theta)$ with various other predictions (see Sec. IV). In Fig. 2 we have compared the



FIG. 2. Supercritical crossover temperatures $K_x(\Theta)$ deduced from the equal-interaction-strength criterion (Sec. III) for dimensions d = 1, 2, 3, 4, 6.

equal-strength crossover lines $K_x(\Theta)$ (evaluated numerically) for d = 1, 2, 3, 4, 6.

IV. DECIMATION RENORMALIZATION GROUP

A decimation RG transformation identical to the type used by BSK (Ref. 2) and by Beale³ on the ϕ^4 model can be applied to the Gaussian model. In *d* dimensions, the canonical configurational partition function is defined by

$$Z_N = \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_N \prod_{\{\vec{i}, \vec{j}\}} \exp[G(x_{\vec{i}}, x_{\vec{j}})],$$
(4.1a)

where

$$G(x,y) = \frac{-1}{2d} [U_1(x) + U_1(y)] - U_2(x,y) ,$$
(4.1b)

$$U_1(x) = \frac{1}{2} \left(\frac{x}{w} \right)^2 - \ln \cosh \left(\frac{xv}{w^2} \right), \qquad (4.1c)$$

$$U_2(x,y) = \frac{1}{2}K(x-y)^2$$
. (4.1d)

This partition function has been evaluated in Secs. II and III. Z_N factorizes into a Gaussian-model partition function and the partition function of an Ising model with exponentially decaying interactions. In one dimension the RG transformation consists of generating a renormalized coupling $\tilde{G}(x,y)$ between the field variables of one sublattice by integrating over the variables at every site of the other sublattice.²¹ This rescales lengths on the lattice by a factor b = 2:

$$e^{\widetilde{G}(x,y)} = \int_{-\infty}^{\infty} dt \exp[G(x,t) + G(t,y)] . \quad (4.2)$$

The advantage of the double-Gaussian model over

the ϕ^4 model is that Eq. (4.2) can be integrated exactly:

$$\widetilde{G}(x,y) = \widetilde{G}(0,0) - \frac{1}{2}(K + \frac{1}{2}w^{-2})(x^2 + y^2) + \frac{1}{2}\ln\cosh\left[\frac{xv}{w^2}\right] + \frac{1}{2}\ln\cosh\left[\frac{yv}{w^2}\right] + \frac{1}{2}K^2w^2(1 + 2Kw^2)^{-1}(x + y)^2 + \ln\cosh\left[\frac{Kv(x + y)}{1 + 2Kw^2}\right], \quad (4.3)$$

where

$$\widetilde{G}(0,0) = \ln \left[\frac{2\pi w^2}{1+2w^2 K} \right]^{1/2} + \frac{v^2}{2w^2(1+2w^2 K)} .$$

 \tilde{G} can then be decomposed into renormalized site potentials and nearest-neighbor couplings:

$$\widetilde{U}_{1}(x) = \left[K + \frac{1}{2}w^{-2} - \frac{2K^{2}w^{2}}{1 + 2Kw^{2}} \right] x^{2}$$
$$-\ln \cosh \left[\frac{xv}{w^{2}} \right]$$
$$-\ln \cosh \left[\frac{2Kvx}{1 + 2Kw^{2}} \right], \qquad (4.4a)$$
$$\widetilde{U}_{2}(x,y) = \frac{\frac{1}{2}K^{2}w^{2}}{1 + 2Kw^{2}}(x - y)^{2}$$

$$-\ln \cosh \left[\frac{Kv (x + y)}{1 + 2Kw^2} \right]$$
$$+ \frac{1}{2} \ln \cosh \left[\frac{2Kvx}{1 + 2Kw^2} \right]$$
$$+ \frac{1}{2} \ln \cosh \left[\frac{2Kvy}{1 + 2Kw^2} \right]. \quad (4.4b)$$

A similar procedure can be applied in 2D with a scale change of $b = \sqrt{2}$.³ If we follow the usual real-space RG methods and truncate the resulting interactions to single-site and nearest-neighbor site potentials, we obtain the following for the renormalization potentials:

$$\begin{split} \widetilde{U}_{1}(x) &= \left[2K + \frac{1}{2}w^{-2} - \frac{8K^{2}w^{2}}{1 + 4Kw^{2}} \right] x^{2} \\ &- \ln \cosh \left[\frac{xv}{w^{2}} \right] \\ &- \ln \cosh \left[\frac{4Kvx}{1 + 2Kw^{2}} \right], \quad (4.5a) \\ \widetilde{U}_{2}(x,y) &= \frac{\frac{3}{2}K^{2}w^{2}}{1 + 4Kw^{2}} (x - y)^{2} \\ &- \frac{3}{4}\ln \cosh \left[\frac{2Kv(x + y)}{1 + 4Kw^{2}} \right] \\ &+ \frac{3}{8}\ln \cosh \left[\frac{4Kvx}{1 + 4Kw^{2}} \right] \\ &+ \frac{3}{8}\ln \cosh \left[\frac{4Kvy}{1 + 4Kw^{2}} \right]. \quad (4.5b) \end{split}$$

The RG procedure then consists of the following steps:

(1) Use Eqs. (3.3a) and (3.3b) to determine v and w from K and Θ .

(2) Insert these values into Eq. (4.5a) or (4.5b) to determine the shape of the renormalized site potential $\tilde{U}_1(x)$. Find out the value \tilde{x}_0 where \tilde{U}_1 has its minimum.

(3) If $\tilde{x}_0 = 0$, the renormalized potential is of Gaussian type, i.e., \tilde{U}_1 has a single-well structure. If $\tilde{x}_0 \neq 0$, then determine the renormalized coupling constants \tilde{K} and $\tilde{\Theta}$ from the equations

$$\frac{\widetilde{K}\widetilde{\Theta}^2}{4(1+\widetilde{\Theta})} = -\widetilde{U}_1(\widetilde{x}_0) , \qquad (4.6a)$$

$$\frac{2\widetilde{K}\widetilde{\Theta}}{1+\widetilde{\Theta}} = \widetilde{U}_2(\widetilde{x}_0, -\widetilde{x}_0) .$$
(4.6b)

These three steps must be done numerically for most of the (K,Θ) parameter space.²²

This procedure gives the Nelson and Fisher¹⁹ (1D) or the Casher and Schwarz⁹ (2D) values for the renormalized coupling constants in the Ising limit. A RG flow pattern for K and Θ can be developed by iterating the transformation. \tilde{K} and $\tilde{\Theta}$ can be fed back into step (1) of the RG procedure to give scale changes of b, b^2, b^4, \ldots Figure 3 shows the phase diagram for the double-Gaussian model in 1D.

Points in the Gaussian region flow to a Gaussian-type high-temperature fixed point under the RG transformation. Points in the disordered Ising region flow to the Ising high-temperature fixed

point at $(K=0, \Theta=\infty)$. Points on the crossover line flow to a fixed point at $(K=0,\Theta\simeq 2)$. As explained in BSK, it is plausible that the crossover line corresponds to the region where the system crosses over from a phonon-dominated region to a domain-wall dominated region. In the Ising region the predominant excitation mode is the formation of domain walls between oppositely ordered regions. This crossover should be accompanied by the appearance of a central peak (at $\omega = 0$) in the dynamic-response function $S(q,\omega)$, although microscopic connections to dynamic quantities⁵ have not yet been made. However, there seem to be definite limitations to the kink-phonon phenomenology in d > 2. The kink-phonon phenomenology for the central peak in $S(q,\omega)$ depends crucially on the appearance of finite clusters of displacements with the same sign. Such clustering occurs in one and two dimensions⁶ so the phenomenology is reasonable in low dimensions. However, for dimensionality d > 2 the block-probability-distribution function is singly peaked for all $T > T_c$.⁶⁻⁸ Presumably for topological reasons, the required clustering does not occur and the kink-phonon phenomenology is questionable at best. This picture of the breakdown of the kink-phonon phenomenology is supported by a recent droplet theory calculation²³ in $1 + \epsilon$ dimensions.

The asymptotic form of the crossover line $K_x(\Theta)$ near $\Theta = 0$ in one dimension is found to be

$$K_{\mathbf{x}}\Theta^{3/2}\simeq \text{const}$$
 (4.7)

in agreement with earlier results^{2,10} and in



FIG. 3. Crossover temperature $K_x(\Theta)$ in one dimension for the double-Gaussian model deduced from decimation RG flows (See Sec. IV).

disagreement with the crossover line derived from the Gaussian-Ising equal-strength criterion [see Eq. (3.17) and subsequent discussion].

Near the Ising limit $(\Theta \rightarrow \infty)$ the RG transformation takes the form

$$\widetilde{K} = \frac{1}{2} \ln \cosh(2K) + \cdots , \qquad (4.8a)$$

$$\widetilde{\Theta} = \frac{K}{\widetilde{K}} \Theta + \cdots \qquad (4.8b)$$

Equation (4.8a) is the exact 1D transformation for the Ising model²¹ with b = 2. Note that $\tilde{K} < K$ for all K so $\tilde{\Theta} > \Theta$. Therefore, all points near enough to the Ising limit ($\Theta \rightarrow \infty$) flow to the Ising limit and infinite temperature.

Figure 4 shows the phase diagram of the 2D double-Gaussian model. Near the Ising limit the RG transformation has the form

$$\widetilde{K} = \frac{3}{8} \ln \cosh(4K) + \cdots , \qquad (4.9a)$$

$$\widetilde{\Theta} = \frac{K}{\widetilde{K}} \Theta + \cdots \quad . \tag{4.9b}$$

Equation (4.9a) is exactly the transformation derived by Casher and Schwartz⁹ for the Ising model. There is a critical fixed point at $(K_c \simeq 0.507, \Theta = \infty)$. The line $K_c(\Theta)$ is the critical line for this model. Points on this line flow into the critical fixed point but with the marginal nature displayed by Eq. (4.9b). Points with $K < K_c(\Theta)$ and sufficiently large Θ flow to the Ising limit and infinite temperture because $\tilde{K} < K$.

Since points on the critical line flow into the Is-



FIG. 4. Critical and crossover temperatures $K_c(\Theta)$ and $K_x(\Theta)$, respectively, for the double-Gaussian model in *two* dimensions deduced from decimation RG flows. (See Sec. IV.) The expected subcritical crossover temperature (Ref. 21) is not shown.

ing critical fixed point, the critical behavior of the system is Ising-type. The critical exponents are, therefore, expected to be the usual Ising exponents in agreement with the Ising nature of the transition derived in Sec. II. At large Θ the critical line has the form

$$K_c(\Theta) \simeq K_c(\infty) + \frac{\text{const}}{\Theta}$$
, (4.10)

in agreement with Sec. III. The RG calculation gives a critical line that is fitted well by a function of the form

$$K_c \Theta \simeq C \ln K_c$$
, (4.11)

for $\Theta \ll 1$. The constant C, however, seems to be in disagreement with Eq. (3.19) by a factor of about 10 and the additional constant term is not present.

The d=2 double-Gaussian model exhibits a crossover line $K_x(\Theta)$ identical in nature to the crossover line in the 1D case. The crossover line divides the disordered region above the critical line into a domain-wall-dominated Ising-type region and a phonon-dominated Gaussian-type region. For small Θ , the crossover line $K_x(\Theta)$ obeys

$$K_x \Theta \simeq C' \ln K_c$$
, (4.12)

with C' a constant. According to an argument in BSK (Ref. 2), we expect that as K is increased at fixed Θ a central peak in $S(q,\omega)$ first appears near $K = K_x(\Theta)$.

So, in 2D as K is increased, at fixed and sufficiently small Θ , the system shows at least²⁴ three types of behavior. At small K the excitations are primarily large-amplitude phononlike oscillations. The particles frequently flip from one side of the double well to the other. There is almost no local ordering. For $K_c > K > K_x$, the system is locally ordered and the dominant excitations are domain walls between oppositely ordered domains. The local structure is of Ising type but with some phonon motion superimposed. Near the critical coupling, long-range ordering sets in, and an Ising-type continuous phase transition occurs. For $K > K_c$ the system is in an Ising-type ordered phase.²⁴

To be complete one should compare the decimation RG scheme used here with the block-spin RG's used⁶ on models of this general type. Blockspin RG's are universal for all models in a given universality class. The fixed points of *decimation* RG's are not universal because even after most of the ordering coordinates have been integrated over, one is still left with single sites of the original lattice. Therefore, the fixed-point potential of a decimation RG will depend sensitively on the precise model in the universality class which is chosen. Even for a given model there is a spectrum of high-temperature fixed points which depend on the parameter (K, Θ , etc.) chosen at the beginning. The infinite-temperature fixed point of a blockspin RG is, however, always a Gaussian model.⁷ Nevertheless, decimation schemes can give universal quantities such as critical exponents correctly and can be a sensitive probe of the local nonuniversal behavior of the chosen system. Not all interesting physical quantities are universal.

V. CONCLUSION

We have presented two alternative ways of investigating the crossover and critical behavior of a displacive-phase-transition model in the Ising universality class. The first method (Secs. II and III) is based on the exact factorization of the double-Gaussian-model partition function into a Gaussian model and an Ising model. From known properties of the Ising model in several dimensions we are able to calculate the location of the critical line near the Ising limit and near the displacive limit. An equal-strength criterion is then used to locate the crossover region in the high-temperature phase. This crossover is from a Gaussian-type region to an Ising-type region with stronger shortrange order from clusters. The second method (Sec. IV) is based on a real-space decimation RG transformation (whose flows are quite different from those of the block-spin RG transformation 6,7) on this same model in one and two dimensions.

We locate the critical and crossover lines by following the trajectories of the renormalized coupling constants. Both calculations give the same functional behavior for the critical and crossover lines in two dimensions. In one dimension the two methods give different functional behaviors for the crossover line $[K_c(\Theta) = \infty$ in one dimension], with the RG method giving the accepted form. However, the qualitative structure of the phase diagram given by the two methods is very similar in the two dimensionalities in which the methods have been compared (1D and 2D). Other thermodynamic properties are being studied, using the simplifications of the double-Gaussian model, and these may shed further light on the phase-diagram details²¹⁻²⁴-we anticipate well-defined but smooth changes in the character of some thermodynamic functions in the neighborhood of the equal-strength crossover.

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in our "displacive" limit (cf. Ref. 19).

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