Renormalization-group study of crossover in structural phase transitions

Paul D. Beale, Sanjoy Sarker,* and J. A. Krumhansl
Laboratory of Atomic and Solid State Physics and Materials Science Center, Cornell University, Ithaca, New York, 14853
(Received 24 October 1980)

The eigenvalues and eigenfunctions of the transfer operator are used to develop an exact renormalization-group (RG) transformation for the ϕ^4 model of structural phase transitions in one dimension. The method we develop is applicable over the entire range from the displacive limit to the order-disorder limit. Analysis of the RG flow near the displacive limit and far from the fixed points enables us to identify a high-temperature Gaussian-like displacive region where phononlike excitations dominate. At lower temperatures a crossover to order-disorder behavior is driven by the formation of domain walls. The transformation is extended to two dimensions by using the Kadanoff-Migdal transformation. A phase diagram is produced, and the displacive region found in one dimension persists. The crossover which occurs above the critical temperature is still identified with the onset of domain-wall formation.

I. INTRODUCTION

A simple microscopic model that has been widely used to describe systems undergoing structural phase transitions[1] is defined by the Hamiltonian

$$H=\frac{1}{2m}\sum_i p_i^2+\sum_i V(x_i)+\frac{C}{2}\sum_{(ij)}(x_i-x_j)^2 \quad . \tag{1}$$

Here (ij) are pairs of nearest-neighbor sites on a d-dimensional hypercubic lattice, and $\{x_i\}$ and $\{p_i\}$ are the displacements and momenta of a set of particles. Each particle is coupled harmonically to its nearest neighbors with interaction strength C. The local potential, V, is of the double-well type:

$$V(x)=-\frac{A}{2}x^2+\frac{B}{4}x^4, \quad B>0 \quad . \tag{2}$$

For $A>0$, V has a pair of minima at $\pm x_0 = \pm (A/B)^{1/2}$. For $d \geq 2$, this system undergoes a second-order phase transition at a critical temperature T_c which is a continuous function of the parameters of the model and vanishes as the double-well character of V disappears, i.e., as $A \rightarrow 0+$.[1]

An interesting parameter in the above model is the ratio of the well depth to the harmonic energy $s=-2V(x_0)/dCx_0^2=(1/2d)A/C$. Traditionally it has been believed[2] that the behavior of the system in the weakly anharmonic displacive regime $s \ll 1$ is qualitatively different from that in the order-disorder regime $s \gg 1$.

Exact results in one dimension[3] and molecular-dynamics studies in higher dimensions[4] indicate that the static and dynamic behavior in the displacive regime has a strong order-disorder character, at least in the critical region, indicating the presence of locally ordered clusters or domains in the system. This is in accord with the universality hypothesis, according to which the model defined by Eqs. (1) and (2) has the same critical behavior as the Ising model. These two models are said to belong to the same universality class. Indeed if we let $A \rightarrow \infty$, $B \rightarrow \infty$, $A/B \rightarrow 1$, the Ising model is recovered from Eqs. (1) and (2). Above the critical temperature the short-range order is expected to persist up to a temperature T_0 above which the system crosses over to a regime where the dominant excitations are anharmonic phonons.

Momentum-space renormalization-group (RG) techniques have been applied to this model in $4-\epsilon$ dimensions[5] and in the displacive limit.[6] More recently,[7] these methods have been used to calculate the probability distribution of block coordinates, lending further support to the hypothesis that the transition has order-disorder character.

In this paper we consider a position space RG transformation on the model. Such methods have been used successfully for discrete spin models, particularly in lower dimensions.[8] Similar transformations for this model have been considered by Bruce and Schneider[9] in one dimension in the displacive regime, and by Burkhardt and Kinzel[10] in the order-disorder regime. Because of the difficulties of carrying out multiple integrations over many variables, the latter authors used an initial restructuring to convert the model into a generalized Ising-like model. Their approximations are not applicable in the displacive regime and, since the Ising universality is built in from the start, the universality properties of the original model are obscured.

Usually RG methods are applied near the fixed points, where the system can be parametrized by a few dominant variables. Away from the critical region, particularly near the crossover region, as we see later, the role of the irrelevant variables becomes

 ©1981 The American Physical Society

physically important. Here we construct an RG procedure which takes into account all of the irrelevant variables exactly. By studying the RG flow diagram in a few variables, we are able to establish the region where the crossover takes place.

We find for one dimension that even though the pseudocritical behavior of the model is always Ising-like for sufficiently low temperatures, the RG flow of the system exhibits two types of noncritical flow behavior. If the well depth is sufficiently deep compared with the interparticle interaction, then the RG flow of the system goes to the Ising high-temperature fixed point. If the well depth is too shallow and if the temperature T is large enough then the RG flow tends to an infinite temperature fixed point which is associated with a system with a Gaussian-like Hamiltonian.

We then use a Kadanoff-Migdal[11] type transformation to generate a two-dimensional RG for this model by using our results from one dimension. This has the advantage that extra interactions (e.g., next-nearest neighbors, etc.), are not generated, so the parameter space is kept small. Even though the Kadanoff-Migdal transformation does not yield accurate estimates of critical exponents, it is expected to provide a quite reliable phase diagram and a good estimate of the critical temperature.

In Sec. II we consider the traditional[12] decimation transformation in one dimension by integrating over every other field variable, yielding a scale change of $b=2$. This is used to derive recursion relations for the parameters in the model near the displacive limit. In Sec. III the decimation procedure is extended to arbitrary scale changes $b \geq 1$ by introducing the transfer operator of the system. This is used to find exact criteria for the crossover from displacive to Ising-like behavior and to generate a RG flow diagram for the entire parameter space of the one dimensional version of this model. In Sec. IV the results from one dimension are used to generate an approximate RG transformation for two dimensions by using a Kadanoff-Migdal transformation. We use this to produce a phase diagram for the two-dimensional system. Concluding remarks are contained in Sec. V.

II. DECIMATION IN ONE DIMENSION

The configurational partition function for the ϕ^4 model defined by Eqs. (1) and (2) is given by

$$Q_N=\int_{-\infty}^{\infty}\prod_i dx_i \exp\left[-\beta\sum_i\left(-\frac{A}{2}x_i^2+\frac{B}{4}x_i^4+\frac{C}{2}(x_i-x_{i+1})^2\right)\right] , \quad (3)$$

where $\beta=(1/k_BT)$. By rescaling the field variables $x_i \rightarrow x_i'=\zeta x_i$, we can eliminate one of the parameters of the model. Therefore the potential energy becomes

$$-\beta U_N=\sum_i\left(\frac{K\theta}{2}x_i^2-\frac{K(\theta+1)}{4}x_i^4-\frac{K}{2}(x_i-x_{i+1})^2\right) , \quad (4)$$

where the dimensionless parameters

$$\theta=A/C , \quad (5a)$$

$$K=\frac{\beta C^2}{B}(1+\theta) , \quad (5b)$$

are independent of ζ. K is an inverse temperature variable which is similar to the one used to parametrize Ising systems. θ is a measure of the displaciveness of the system. For fixed K, as $\theta \rightarrow 0+$ the double well vanishes. We will call this the displacive limit. As $\theta \rightarrow \infty$ the well depth diverges and therefore the field variables x_i become confined to the regions near $\pm x_0=\pm[\theta/(\theta+1)]^{1/2}$. This is the Ising limit. This particular parametrization is chosen so that even at the displacive limit the quartic term in Eq. (4) is positive, ensuring that the particles remain localized near their lattice sites. A somewhat different form of parametrization is used by some other authors.[1]

To define a RG transformation in one dimension we rewrite Eq. (3) in the form

$$Q_N=\zeta^N\int_{-\infty}^{\infty}\prod_i dx_i \exp[G(x_i,x_{i+1})] , \quad (6)$$

where

$$G(x,y)=K\left(\frac{\theta}{4}(x^2+y^2)-\frac{\theta+1}{8}(x^4+y^4)-\frac{1}{2}(x-y)^2\right) . \quad (7)$$

Following the standard decimation scheme,[12] a real space RG procedure can be carried out by integrating over every other field variable.

$$\int_{-\infty}^{\infty} du \exp[G(x,u)+G(u,y)]=\exp[g_0+\tilde{G}(x,y)] . \quad (8)$$

This yields a new function $\tilde{G}$ which also has couplings only between nearest neighbors.

g_0 is chosen so that $\tilde{G}(0,0)=0$. It is an analytic function of the parameter (K,θ) and is important in the calculation of the free energy per particle but does not affect the critical properties of the system. The above thinning out of the degrees of freedom rescales all lengths in the system by a factor $b^{-1}=\frac{1}{2}$. The next step is to rescale the field variables $x_i \rightarrow x_i'=\tilde{\zeta}x_i$ with a suitable choice of $\tilde{\zeta}$. Since $\tilde{G}$ couples only nearest-neighbor variables, the procedure can be repeated until G reaches a fixed functional form G^*. In practice such an iteration procedure is

difficult to carry out analytically because $\tilde{G}$ does not have the same simple form as G. To see this, substitute Eq. (7) into Eq. (8) and obtain

$$\exp[g_0+\tilde{G}(x,y)]=\exp\left[K\left(\frac{\theta-2}{4}(x^2+y^2)-\frac{\theta+1}{8}(x^4+y^4)\right)\right]\left(\frac{4}{K(\theta+1)}\right)^{1/4} f\left(\left(\frac{4K^3}{1+\theta}\right)^{1/4}(x+y)\right) , \tag{9}$$

where

$$f(z)=\int_{-\infty}^{\infty} du\,\exp(-2pu^2-u^4+zu) , \tag{10}$$

$$2p=(2-\theta)\left(\frac{K}{\theta+1}\right)^{1/2} . \tag{11}$$

The function $f(z)$ cannot in general be replaced by a function of the form $\exp(\alpha z^2-\gamma z^4)$. However for one region of the (K,θ) parameter space it is valid to expand $f(z)$ in a power series. In this region ($\theta^{-2} \gtrsim K \gtrsim 2$), one can cut off the power series after the quartic term in z. By carefully identifying terms and ignoring anharmonic bond terms of the form $(x^2-y^2)^2$ and $(x-y)^4$ we get the following recursion relations first obtained by Bruce and Schneider[9]:

$$\tilde{\theta}=4\theta-\theta^2+\cdots , \tag{12}$$

$$\tilde{K}^{-1}=8K^{-1}+\cdots . \tag{13}$$

There is a fixed point at $\theta^*=0$, $K^*=\infty$, which is doubly unstable with eigenvalues $\lambda_1=3$, $\lambda_2=2$. This crossover leads to drastically different behavior on the lines $\theta=0$ and $K=\infty$. For K sufficiently large, the system maps onto the Ising model at low temperature (as will be shown in Sec. III). On the $\theta=0$ line, the system has no possibility of a spontaneous symmetry breaking because of the monotonic nature of the one-particle potential in this limit. The system exhibits no pseudocritical behavior on this line.

The crossover between the two different types of behavior is describable by a crossover scaling function $Y=Y(K^{-1}\theta^{-\lambda_1/\lambda_2})$. Therefore one can divide the two regions by the curve $K\theta^{3/2}=\text{const}$ which defines a temperature $T_0(\theta)=\text{const}\,\theta^{3/2}$. To see the significance of this we can make contact with the exact calculations of Krumhansl and Schrieffer.[3] They find important low-energy excitations, domain walls, which play a crucial role in the statics and dynamics of this one-dimensional system at low temperatures. The picture is as follows. At zero temperature, for any positive θ, the system is perfectly ordered; i.e., all of the particles sit at the bottom of one side of all the wells. This order is broken at nonzero temperatures by the formation of domain walls, so that there is no long-range order in one dimension for any $T>0$. Nevertheless, the density of these domain walls is rather small at low temperatures, being proportional to $\exp(-\beta E_D)$, where E_D is the energy of a domain wall. As long as $k_BT \ll E_D$, large regions of nearly perfectly ordered clusters exist in the system even though there is no long-range order. The existence of these clusters provides one model for an important dynamical effect, namely, the central peak in the dynamic response function, attributable to the slow fluctuations of the local order parameter within the clusters.

When $k_BT \approx E_D$ the density of domain walls increases rapidly with temperature and the central peak disappears. We can define a crossover temperature T_0 which signals the onset of short-range order (formation of clusters). Since, from Krumhansl and Schrieffer,[3] $E_D \propto \theta^{3/2}$, we find $T_0 \propto \theta^{3/2}$ in agreement with the RG prediction.

The recursion relations (12) and (13) are valid only for $\theta^{-2} \gtrsim K \gtrsim 2$, since the truncation of the power series expansion of Eq. (9) is not valid outside this region. Outside this region higher and higher powers of $(x+y)$ become significant. This means that the parameter space must be enlarged, which in turn makes the problem analytically intractable. Even in the truncated problem the anharmonic bond terms were ignored arbitrarily. We can avoid these difficulties using an alternative formulation of the problem which we now discuss.

III. DECIMATION IN ONE DIMENSION USING THE TRANSFER OPERATOR

An alternative realization of the RG transformation can be obtained by using the transfer integral techniques of Scalapino, Sears, and Ferrell.[13] This method uses the fact that, in one dimension, $e^{G(x,y)}$ can be expanded exactly in terms of a certain complete set of functions, i.e.,

$$e^{G(x,y)}=\sum_{n=0}^{\infty}\lambda_n\phi_n(x)\phi_n(y) ,$$

where $\{\phi_n\}$ and $\{\lambda_n\}$ are the eigenfunctions and eigenvalues of the integral equation

$$\int_{-\infty}^{\infty} dy\,\exp[G(x,y)]\phi_n(y)=\lambda_n\phi_n(x) . \tag{14}$$

We choose the eigenfunctions to be normalized and, as we show later, they are guaranteed to be orthogonal and complete, i.e.,

$$\int_{-\infty}^{\infty} dx\,\phi_n(x)\phi_m(x)=\delta_{nm} , \tag{15}$$

$$\sum_{n=0}^{\infty}\phi_n(x)\phi_n(y)=\delta(x-y) . \tag{16}$$

To see the advantage of the representation (14), let us integrate out $b-1$ out of every b spins. The resulting $\tilde{G}_b$ function is then given by

$$\exp[g_0+\tilde{G}_b(x,y)]=\int_{-\infty}^{\infty}du_1\cdots\int_{-\infty}^{\infty}du_{b-1}\exp[G(x,u_1)+\cdots+G(u_{b-1},y)]=\sum_{n=0}^{\infty}\lambda_n^b\phi_n(x)\phi_n(y)\ . \tag{17}$$

The advantage of Eq. (17) is that we can let the decimation factor b assume any value greater than or equal to 1, discrete or continuous. In particular, $\tilde{G}_1(x,y)=G(x,y)$ (i.e., no decimation), and $\tilde{G}_2(x,y)=\tilde{G}(x,y)$ used in Sec. II. By letting $b=1+\epsilon$ with $\epsilon \ll 1$, an infinitesimal (i.e., differential) RG transformation can be generated. More importantly, Eq. (17) allows us to avoid the problems encountered by the direct integration method used in Sec. II. Usually b is taken to be a small integer, say 2 or 3. The resulting $\tilde{G}_b$ function is usually much more complicated than the original one. One then approximates $\tilde{G}_b$ by replacing it with some simpler function with the implicit assumption that the neglected terms (e.g., the anharmonic bond terms in Sec. II) are irrelevant. This is an uncontrolled approximation since it is not obvious *a priori* whether or not after many iterations such irrelevant terms feed back into the relevant ones to make a significant difference. From Eq. (17) we see that we can bypass this difficulty since we can iterate many times simply by increasing b. This involves no approximation at all. Thus we can study the scaling of the entire $\tilde{G}_b$ function as b increases.

For $K>0$ the kernel of Eq. (15) generates a positive definite, symmetric, Hilbert-Schmidt linear operator. Therefore we know that the eigenfunctions are square integrable and form a complete set, eigenfunctions associated with different eigenvalues are orthogonal and

(a) $\lambda_n>0$ for all λ ,

(b) $\lim_{n\to\infty}\lambda_n=0$,

(c) $\sum_{n=0}^{\infty}\lambda_n<\infty$.

Furthermore, since the kernel is positive for all $|x|,|y|<\infty$ (as long as $K<\infty$), the eigenvalue spectrum is nondegenerate so we can order the eigenvalues

(d) $\lambda_0>\lambda_1>\lambda_2>\lambda_3>\cdots>0$,

and because $G(-x,-y)=G(x,y)$ the eigenfunctions have the property

(e) $\phi_n(-x)=(-1)^n\phi_n(x)$.

It is easy to see from this that there are no RG fixed points for a system of this type of any K in the range $0<K<\infty$. This is just a reflection of the fact that no one-dimensional system with short-range forces can have long-range order. However, fixed points can reside on the lines $K=0$ and ∞. In particular, for any $K<\infty$, when the RG scale factor b is taken large enough, the coupling between adjacent particles can be made as small as desired, i.e.,

$$\lim_{b\to\infty}[g_0+\tilde{G}_b(x,y)]=b\ln\lambda_0+\ln\phi_0(x)+\ln\phi_0(y)+\left[\frac{\lambda_1}{\lambda_0}\right]^b\frac{\phi_1(x)\phi_1(y)}{\phi_0(x)\phi_0(y)}+\cdots\ , \tag{18}$$

where the ellipsis represents higher-order terms. This means that the renormalized temperature is tending to ∞ as $b\to\infty$, and thus flows to some high-temerature fixed point.

On the other hand, near $T=0$ ($K\to\infty$), for any $\theta>0$, the only contribution to Eq. (15) comes from the neighborhood of $\pm x_0=\pm[\theta/(\theta+1)]^{1/2}$ (the bottom of the wells). Then it is not difficult to show that the eigenfunctions associated with the largest two eigenvalues are essentially given by linear oscillator ground states centered at the bottom of each well

$$\psi_{\pm}(x)\cong\frac{L}{\sqrt{2}}\{\exp[-\alpha(x-x_0)^2]\pm\exp[-\alpha(x+x_0)^2]\}\ , \tag{19}$$

where

$$\alpha\approx\frac{K}{2}[\theta(\theta+2)]^{1/2}\ . \tag{20}$$

L is a normalization constant and α diverges as $K\to\infty$. The eigenvalues are given by

$$\lambda_{\pm}=\exp[-(\epsilon_0\pm t)]\ , \tag{21}$$

where

$$\epsilon_0\approx\frac{K\theta^2}{8(\theta+1)}+\frac{1}{2}\ln\left[\frac{\pi}{K\{1+\theta+[\theta(\theta+2)]^{1/2}\}}\right]\ , \tag{22a}$$

$$t\approx\exp(-\beta E_D)\ . \tag{22b}$$

The quantity E_D is the domain-wall energy and is independent of temperature. As $K\to\infty$ (i.e., $T\to0$) the two states become asymptotically degenerate, signaling the onset of a phase transition. Thus to obtain the fixed point function we must retain both of these states in Eq. (17). In this limit the states (19) reduce to the sum and difference of δ functions, so the

model maps onto the Ising model at low temperatures. This shows that the critical behavior of this model is identical to that of the Ising model.

Since the functions $\tilde{G}_b$ do not have the same functional form as G, some method other than the one used in Sec. II must be devised in order to define the recursion relations for K and θ. Let us first define the renormalized one-particle and two-particle couplings $\tilde{U}_1^{(b)}$ and $\tilde{U}_2^{(b)}$ by

$$\tilde{G}_b(x,y) = -\tfrac{1}{2}[\tilde{U}_1^{(b)}(x) + \tilde{U}_1^{(b)}(y)] - \tilde{U}_2^{(b)}(x,y) \ . \tag{23}$$

Of course for $b=1$ these functions reduce to the original forms:

$$\tilde{U}_1^{(1)}(x) = -\frac{K\theta}{2}x^2 + \frac{K(\theta+1)}{4}x^4 \ , \tag{24}$$

$$\tilde{U}_2^{(1)}(x,y) = \frac{K}{2}(x-y)^2 \ . \tag{25}$$

From numerical work to be described later, we observe that for most of the (K,θ) parameter space the function $\tilde{U}_1^{(b)}$ has minima at $\pm\tilde{x}_0$ and looks qualitatively like $\tilde{U}_1^{(1)}$. We therefore define the renormalized coupling constants $(\tilde{K}_b, \tilde{\theta}_b)$ and the rescaling factor $\tilde{\zeta}_b$ by

$$\tilde{\theta}_b = \frac{8\tilde{U}_1^{(b)}(\tilde{x}_0)}{\tilde{U}_2^{(b)}(\tilde{x}_0,-\tilde{x}_0)} \ , \tag{26}$$

$$\tilde{K}_b = \frac{1}{2}\left[\frac{\tilde{\theta}_b+1}{\tilde{\theta}_b}\right]\tilde{U}_2^{(b)}(\tilde{x}_0,-\tilde{x}_0) \ , \tag{27}$$

$$\tilde{\zeta}_b = \tilde{x}_0^2\left[\frac{\tilde{\theta}_b+1}{\tilde{\theta}_b}\right] \ . \tag{28}$$

The points $\pm\tilde{x}_0$ are the x values where $\tilde{U}_1^{(b)}$ has its minima. This method ensures that the renormalized coupling function $\tilde{G}_b$ is exactly correct at the points $(x,y) = [(0,0), (\tilde{x}_0, \pm\tilde{x}_0)]$. For $b=1$, these definitions reduce to the original form. For $b>1$ a "ϕ^4" potential parametrized by $(\tilde{K}_b, \tilde{\theta}_b)$ agrees with the true renormalized coupling at the top and bottom of the wells.

This definition of the renormalized coupling constants is certainly valid near the Ising limit because there the field variables x_i can only have the values $\pm x_0$. In fact an asymptotic expansion of Eq. (10) for large θ gives the exact Ising RG recursion relation for K, plus correction terms of order $1/\theta$ when these definitions are used. It is not obvious *a priori* that these definitions are valid for small values of θ (except in the region discussed in Sec. II) or for $\theta \approx 1$. Figures 1(a) and 1(b) show the quality of this fit for $K=6.0$, $\theta=0.45$, $b=2$. Figure 1(a) shows the exponential of the one-particle coupling obtained from Eqs. (17) and (24) plotted over the fitted function using the parameters $(\tilde{K}_b, \tilde{\theta}_b, \tilde{\zeta}_b)$ defined by Eqs. (26)–(28). Figure 1(b) shows the corresponding points for the two-particle coupling. This is a quite satisfactory fit considering the abundance of high-order terms which appear in the true renormalized couplings. Other regions of the parameter space give equally satisfactory fits.

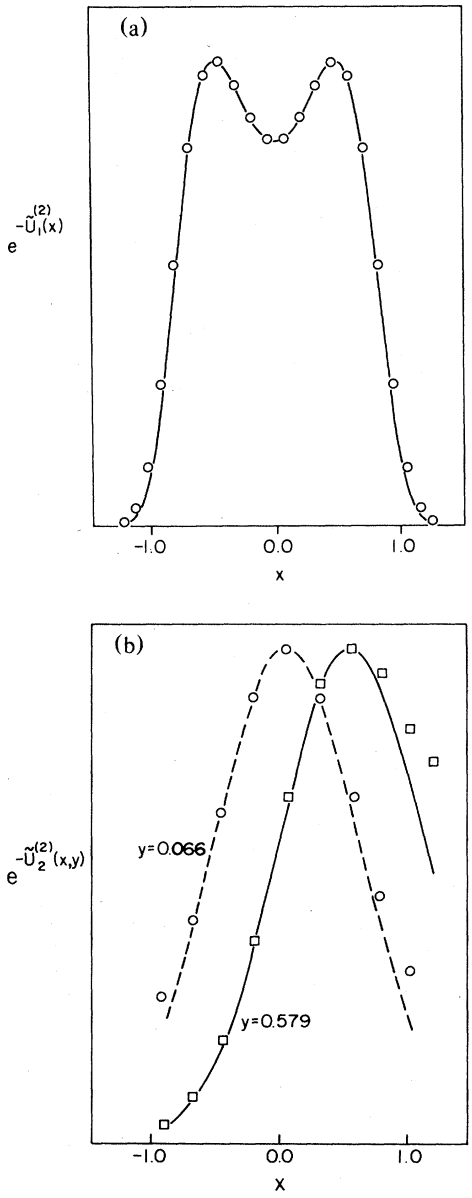

FIG. 1. Renormalized one-particle and two-particle couplings for $K=6.0$, $\theta=0.45$, $b=2$. The circles and squares are exact and the solid and dashed lines result from fitting the exact couplings at the top and bottom of the double-well single-particle potential.

The numerical calculation of the renormalized couplings is accomplished by the following method.[14]

We approximate the integral eigenvalue equation (14) by

$$\sum_{j=1}^{N} w_j \exp[G(x_i,x_j)]\phi_n(x_j) = \lambda_n \phi_n(x_i) \ , \qquad (29)$$

where (w_j) and (x_j) are the Gaussian integration formula weights and abscissa points, respectively.[15] By multiplying both sides of Eq. (29) by $(w_i)^{1/2}$ we get

$$\sum_{j=1}^{N} T_{ij}\phi_j^{(n)} = \lambda_n \phi_i^{(n)} \ , \qquad (30a)$$

where

$$T_{ij} = (w_i w_j)^{1/2} \exp[G(x_i,x_j)] \ , \qquad (30b)$$

$$\phi_j^{(n)} = (w_j)^{1/2}\phi_n(x_j) \ . \qquad (30c)$$

Now the problem has been reduced to finding the eigenvalues and eigenvectors of a real, symmetric, $N \times N$ matrix. This is easily accomplished by using standard computer routines.

Once the eigenfunctions are determined at the N points, very accurate estimates of the eigenfunctions at all points can be determined by

$$\phi_n(x) = \frac{1}{\lambda_n} \sum_{j=1}^{N} w_j \exp[G(x,x_j)]\phi_n(x_j) \ . \qquad (31)$$

The bulk of our results, the RG flow pattern of the system in the parameters K and θ for one dimension, are displayed in Figs. 2(a) and 2(b). Figure 2(a) is produced by starting at some initial points (K, θ) and performing the summation (17) with the eigenvalues and eigenfunctions of Eq. (15) for many values of $b(b_0, b_0^2, b_0^4, \ldots, b_{\text{final}})$. Then we use Eqs. (26)–(28) to find the renormalized coupling constants $(\tilde{K}_b, \tilde{\theta}_b)$ for all these values of b. This is hereafter called method I. Figure 2(b) is produced by starting with (K, θ) and performing the above RG transformation with $b = b_0$. We than start all over again using $(\tilde{K}_{b_0}, \tilde{\theta}_{b_0})$ in place of (K, θ) in $G(x,y)$. This procedure is iterated n times to get a system whose scale has been changed by $b_{\text{final}} = b_0^{2^n}$. This will be called method II.

If these two methods give sensibly the same values of $(\tilde{K}_{b_{\text{final}}}, \tilde{\theta}_{b_{\text{final}}})$ for the same initial point then we can safely assume that we have not left out any relevant terms from our calculation, i.e., replacing G by a ϕ^4 form is valid. Therefore either procedure discussed above constitutes a valid means of defining recursion relations for the system.

However, if grossly different $(\tilde{K}_{b_{\text{final}}}, \tilde{\theta}_{b_{\text{final}}})$ result from these two methods then some relevant parameter has been omitted inadvertently. In this case the RG recursion relations must be supplemented by recursion relations for this additional parameter.

In the present case both methods give qualitatively

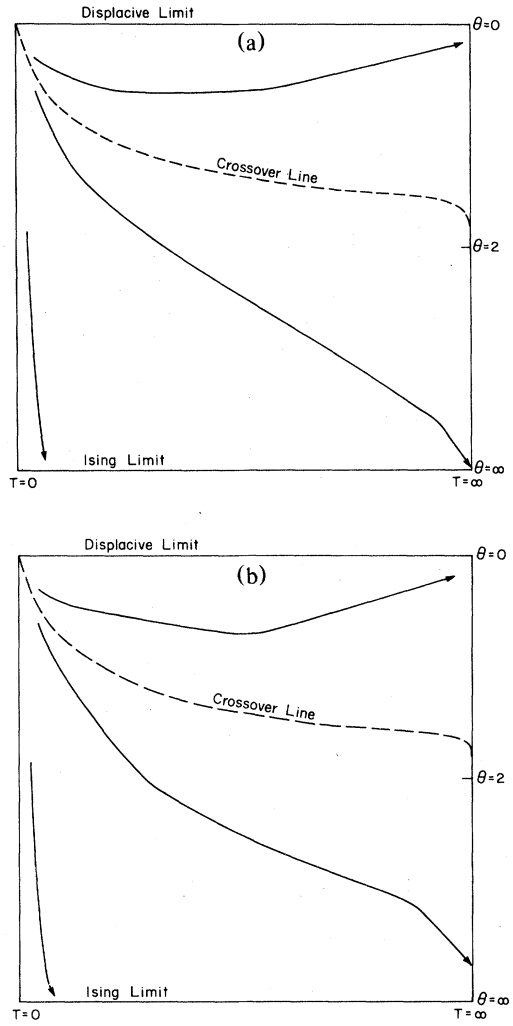

FIG. 2. RG flow for the one-dimensional ϕ^4 model. Method I is depicted in (a) and method II in (b). The area above the crossover line is the high-symmetry displacive region and the area below the crossover line is the order-disorder Ising-like region. $\tanh(1/4K)$ is plotted vs $1-\tanh(\theta/4)$.

the same results over most of the parameter space of the model [Figs. 2(a) and 2(b)]. Both show a dichotomy of flow separated by a sharp crossover line. All points (K, θ) which start below the crossover line eventually flow to the Ising high-temperature fixed point.

All points which start above the crossover line flow to a high-temperature fixed point which is distinct from the Ising high-temperature fixed point. This fixed point, as will be seen shortly, is associated with a model Hamiltonian which exhibits a Gaussian-like symmetry. Since we are discussing a one-dimension-

al system, this divergence of flow is not associated with critical behavior. It does, however, cast some light on the nature of the short-range order of the system and of the form expected for the correlation functions away from T_c.

Figures 3(a) and 3(b) show the shape of the one-particle potential $\tilde{U}_1^{(b)}(x)/\tilde{K}_b$ for several values of b. The two figures depict the difference between the behavior of two points which start on opposite sides of the crossover line. This is not a fit, but the actual couplings generated from Eqs. (17) and (24). In Figure 3(a) the system starts at a point just below the crossover line. Note how the well depth increases dramatically as b increases. Figure 3(b) depicts a system which started just above the crossover line. The well depth increases slightly and then goes rapidly to zero. For b large enough the potential becomes monotonic and similar in form to the Gaussian model. A system with a one-particle potential of this sort has no possibility of having a spontaneously broken symmetry, even in higher dimensions.

Using method I, a precise criterion for the crossover line can be derived. From Eqs. (18) and (23) we see that as $b \to \infty$

$$\tilde{U}_1^{(b)}(x) \approx -\ln\left[\frac{\phi_0(x)}{\phi_0(0)}\right] + O\left(\left[\left(\frac{\lambda_1}{\lambda_0}\right)^b\right]\right) . \tag{32}$$

For large b the one-particle coupling depends only on $\phi_0(x)$. From an examination of the possible solutions of Eq. (15) we find that $\phi_0(x)$ is positive definite, even in x, and has at most two local maxima. Therefore either $U_1^{(b\to\infty)}$ has two minima at $\pm\tilde{x}_0$ or it has only a single minimum at the origin. In the former case the one-particle potential maintains the symmetry of the Ising model. Since the interparticle coupling tends to zero for large b, θ_b is proportional to the well depth divided by the interparticle coupling, which approaches ∞. The coupling constants flow to $(K=0, \theta=\infty)$, the Ising high-temperature fixed point.

$\tilde{U}_1^{(b\to\infty)}(x)$ has two minima if and only if the quantity

$$\frac{\phi_0''(0)}{\phi_0(0)} = K\left[\frac{\theta}{2} - 1 + K\left[\frac{\int dy\, y^2 \exp[G(0,y)]\phi_0(y)}{\int dy \exp[G(0,y)]\phi_0(y)}\right]\right] \tag{33}$$

is positive. One can instantly see that this is always satisfied for $\theta > 2$. All systems with $\theta > 2$ therefore flow to the Ising high-temperature fixed point. For $\theta < 2$ we find that there is always a nonzero range of K such that the inequality (33) is not satisfied. In that region the RG flow is to the displacive high-temperature fixed point. There is a fixed point at $(K=0, \theta=2)$ which sharply divides the two regions.

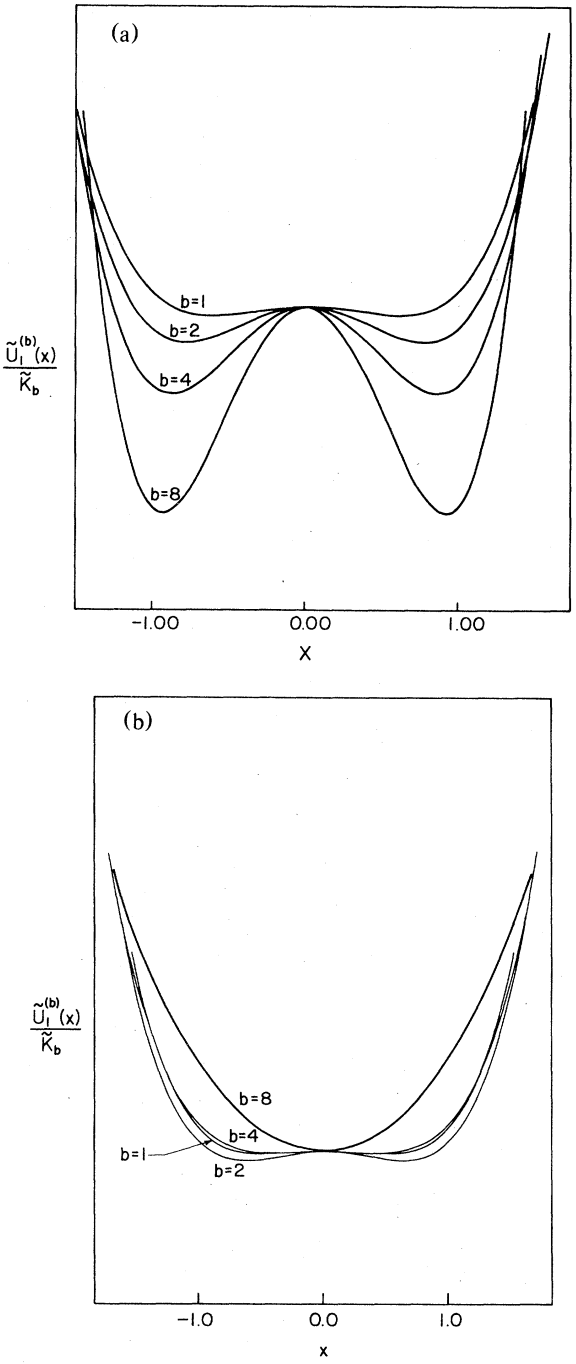

FIG. 3. Shape of the renormalized one-parucle potential is shown for various values of the scale change factor b. In (a) the starting value of (K, θ) is $K=6.0$, $\theta=0.6$, which is just inside the order-disorder region. The well depth increases without limit as $b \to \infty$. In (b) the starting values are $K=6.0$, $\theta=0.3$, which lies just inside the displacive region. The well depth vanishes for $b \geq 4.29$. $\tilde{U}_1^{(b)}(x)$ is well behaved and tends to a fixed form as $b \to \infty$. The increasing well depth in (a) reflects the fact that the ratio of the well depth to the interparticle strain energy diverges as $b \to \infty$.

The locus of points such that the quantity (33) is set equal to zero is the dotted line in Fig. 2(a). This defines the crossover line between the two types of flow behavior. For $\theta >> 1$, these points are numerically consistent with the relation $K\theta^{3/2} = \text{const}$, in agreement with the analysis in Sec. II.

One might note here that $\phi_0^2(x)$ is precisely the one-particle probability distribution function $P_1(x)$ for the one-dimensional model. Bruce, Schneider, and Stoll[7] use the disappearance of double maxima in a *block-spin* probability distribution to signal the onset of displacive behavior. In two dimensions, phonon contributions mask the appearance of double maxima in $P_1(x)$, but by averaging over several nearby sites the double peak structure of the block probability distribution function reemerges.

Very near the crossover line, methods I and II give drastically different RG flows, especially near the fixed point at $(K=0,\ \theta=2)$ because the crossover lines do not coincide exactly. If methods I and II are applied to the same point (K, θ) near the crossover line the RG flows may go to different fixed points. So in this region the RG recursion relations we have constructed do not consititue a semigroup (i.e., if R_b is the RG operator, $R_{b'}R_b \neq R_{bb'}$). Two parameters are not sufficient to describe the flow completely. Two parameter scaling is not valid in this region. Elsewhere in the parameter space the two methods agree very well, two parameter scaling is valid, and the recursion relations we have defined constitute a valid RG.

IV. EXTENSION TO TWO DIMENSIONS: THE KADANOFF-MIGDAL TRANSFORMATION

It is not easy to extend our formalism to higher dimensions since the one-dimensional transfer integral is of limited use. However, the Kandanoff-Migdal[11] transformation is tailored to take advantage of the exact nature of the one-dimensional results and has had some success in providing reliable phase diagrams, particularly in two dimensions.[11] Also, as was shown by Kadanoff, the transition temperature is given correctly in two dimensions for the Ising and Potts models since the Kadanoff-Migdal transformation commutes with the duality transformation. The similarity of the system under consideration here to the Ising model suggests that at least for large θ one may expect the transformation to give reliable estimates for T_c. In what follows we adopt a version of Kadanoff's bond moving scheme to study the behavior of the system.

We start by associating with every bond [Fig. 4(a)] of a square lattice an interaction of the form

$$G(x,y) = K\left[\frac{\theta}{8}(x^2+y^2) - \frac{\theta+1}{16}(x^4+y^4) - \frac{1}{2}(x-y)^2\right] . \tag{34}$$

Notice that the local term differs from the corresponding term in one dimension by a factor of 2 since every such term in the Hamiltonian is divided into the four bonds at each site. The decimation is effected by first moving $b-1$ out of every b vertical bonds as shown in Fig. 4(b). The field variables at the lattice points marked by crosses are then connected with their neighbors only along the horizontal directions and therefore can be integrated out using the methods of Sec. III. Denoting the horizontal and vertical interactions by G_x and G_y, respectively, we obtain [Fig. 4(c)]:

$$\exp[G_x'(u,v)] = \sum_{n=0}^{\infty} \lambda_n^b(K,\theta)\phi_n(u;K,\theta)\phi_n(v;K,\theta) \tag{35}$$

and

$$G_y'(u,v) = bG_y(u,v) = G_y(u,v;bK,\theta) . \tag{36}$$

The standard procedure is to rotate the lattice by 90° and repeat the operation, which gives

$$\exp[G_x''(u,v)] = \exp[bG_x'(u,v)] = \left[\sum_n \lambda_n(K,\theta)\phi_n(u;K,\theta)\phi_n(v;K,\theta)\right]^b , \tag{37}$$

$$\exp[G_y''(u,v)] = \sum_n \lambda_n^b(bK,\theta)\phi_n(u;bK,\theta)\phi_n(v;bK,\theta) . \tag{38}$$

The new interactions G_x'' and G_y'' are usually not equal even if the starting interactions are isotropic, except when b is infinitesimally close to unity. To make the new interactions isotropic we just take the average of G_x'' and G_y'', i.e.,

$$\tilde{G}(u,v) = \tfrac{1}{2}[G_x''(u,v) + G_y''(u,v)] . \tag{39}$$

For $b \to 1+$, this averaging does not change the resulting couplings. For $b > 1$ but small, the change in the critical parameters (e.g., T_c) is small. For example, applying this procedure with $b=2$ to the Ising model gives $K_c = 0.429$, which is within 3% of the exact value $K_c^{\text{exact}} = 0.4407$.

The Kadanoff-Migdal transformation can be applied to the ϕ^4 model (1) in two dimensions by using Eqs. (35)–(39) and finding the renormalized coupling constants by methods similar to those used in

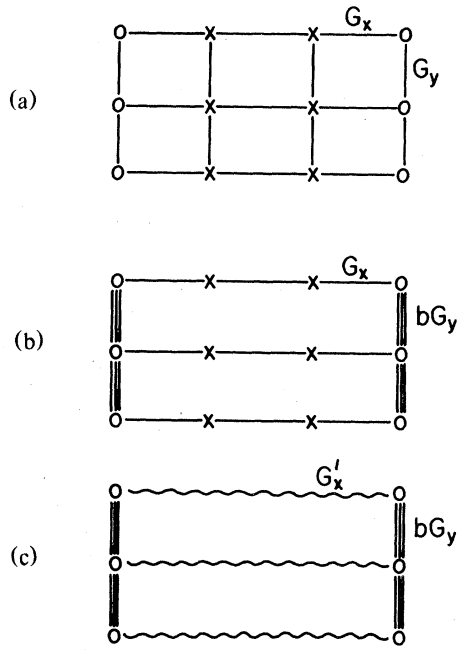

FIG. 4. Kadanoff-Migdal scheme for creating an approximate RG in two dimensions. The case with $b=3$ is illustrated.

Eqs. (26)–(28) in Sec. III. Since the Kadanoff-Migdal transformation works best for b close to 1 we use only method II (i.e., repeated decimation) to produce the RG flow of the system. Figure 5(a) shows the RG flow using a step size of $b=2$. The most obvious difference from the one-dimensional RG flow diagram is the appearance of a critical manifold, $K_c(\theta)$, i.e., a locus of points $K_c(\theta)$ that flow to the fixed point at $\theta=\infty$ and $K_c(\infty)=0.429$. Since the coupling is finite there, this is the critical fixed point corresponding to the Ising critical point. Since the RG flow of points near the critical line goes by the Ising critical point, the critical exponents of the ϕ^4 model $0<\theta<\infty$ are identical to those of the Ising model. We find numerically that $K_c(\theta)\approx\text{const}\,[(\theta+1)/\theta]$ for all $0<\theta<\infty$. This just means that the critical temperature is proportional to the intersite strain energy, which has been shown rigorously for dimensionality $d\geq 3$.[1]

For $\theta>>1$, the critical temperature departs from the Ising value linearly in $1/\theta$. For $\theta<<1$ the reduced critical temperature $T_c(\theta)=1/Kc$ is given by

$$T_c\cong 0.8\theta,\quad \theta<<1\ . \tag{40}$$

Another feature of the RG flow diagram is the persistence of nonuniversal flow [points (K,θ)] which flows into the displacive high-temperature fixed point. For small θ crossover line $T_0(\theta)$ takes the

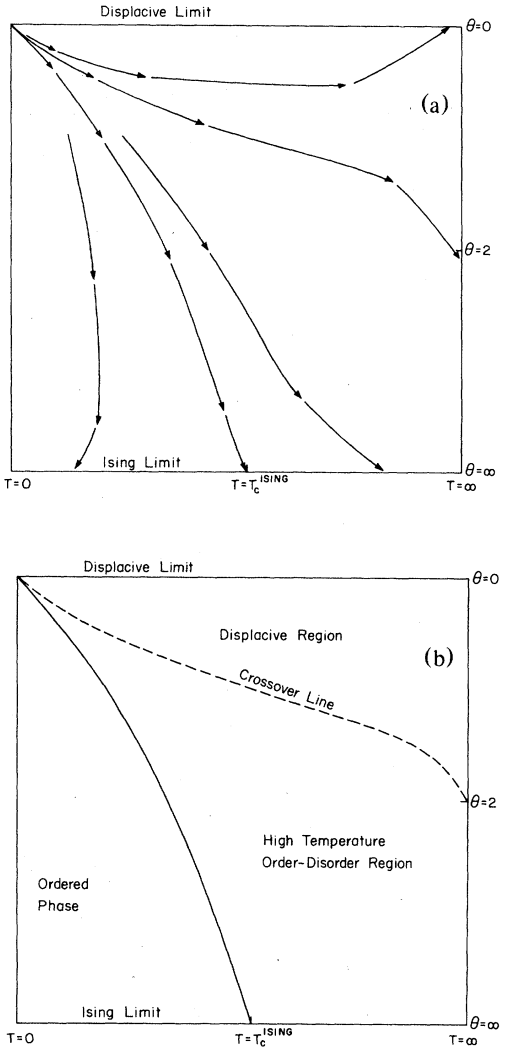

FIG. 5. RG flow (a) and "phase diagram (b) for the ϕ^4 model in two dimensions using the Kadanoff-Migdal transformation. The scales used are identical to Figs. 2(a) and 2(b).

form

$$T_0(\theta)\cong 1.2\theta,\quad \theta<<1\ . \tag{41}$$

This is in agreement with the result of applying the Kadanoff-Migdal transformation to the recursion relations (12) and (13) near the displacive limit. This gives a crossover exponent of $\lambda_1/\lambda_2=1$ so the crossover line is predicted to be

$$\frac{T_0}{\theta}=\text{const}\ . \tag{42}$$

By using the same identification of the meaning of this crossover used in Sec. III, we find that the onset of domain-wall formation occurs for temperature T_0

such that $T_0 \cong 1.3 T_c$. By using this identification, it is plausible that for $T > T_0(\theta)$ the primary excitations of the system are phononlike oscillations about the top of the well. As the temperature is lowered to T_0, domain walls form around regions of the size of the correlation length. At $T = T_c(\theta)$ the system undergoes a continuous phase transition into an ordered state. The critical exponents take on the Ising values of $\alpha = 0$ (log), $\beta = \frac{1}{8}$, $\gamma = \frac{7}{4}$, etc.

For $\theta \gtrsim 2$ the primary excitation mode of the system is domain-wall formation. The effect of phonons is small because the well depth is too big to allow thermal excitations between wells except very infrequently. The system is Ising-like for all temperatures. For $\theta << 1$ the system is Ising-like below T_c, where the system is ordered, and the Ising-like behavior persists above the critical temperature for a small range $T_0 - T_c \approx 0.3 T_c$. In that region the dominant excitations are domain walls separating regions of opposite signs of the order parameter. Above the crossover temperature T_0 the domain walls begin to disappear and the dominant excitations are phonon oscillations about the center of the one-particle potentials.

The crossover from displacive to order-disorder behavior can be observed experimentally by the appearance of a central peak at $\omega = 0$ in the dynamic response function $S(q, \omega)$. For T above T_0 the response function would have peaks at $\omega = \pm\omega_q$ corresponding to phonon oscillations. The peaks are widened due to the nonlinearities in the Hamiltonian. As T is lowered to the crossover temperature T_0 domains of oppositely ordered particles form. Note well that this is a *local* ordering phenomenon only and no long-range correlations are present. The domain walls move around due to the inherent dynamics of the system and due to random thermal fluctuations. Occasionally a particle will be flipped from one side of its well to the other in addition to performing phonon oscillations. The effect of these two processes on $S(q, \omega)$ can be described phenomenologically following the analysis of Krumhansl and Schrieffer.[3] For q^{-1} less than the average distance between domain walls they find

$$S(q,\omega) \sim \sigma(q)\left[x_0^2 \frac{t_D}{1+4\omega^2 t_D^2} + \bar{\alpha}^2\left[\frac{t_D}{1+4(\omega-\omega_q)^2 t_D^2} + \frac{t_D}{1+4(\omega+\omega_q)^2 t_D^2}\right]\right], \tag{43}$$

where t_D is the average time between passages of domain walls, $\bar{\alpha}^2$ is the average squared phonon amplitude, and $\sigma(q)$ is the spatial Fourier transform of x_i over a correlation length (approximately equal to the distance between domain walls). The central peak appears naturally as soon as the domain size becomes appreciable. Since t_D is proportional to the average domain size, the width of the central peak decreases and the height increases as the critical temperature is approached.

There is no effect on the small q (q^{-1} correlation length) behavior of $S(q, \omega)$ or the long-range ($r \gtrsim$ correlation length) behavior of the equal time correlation functions in the crossover region because the formation of domain walls is a local phenomenon only.

Recent molecular-dynamics simulations by Schneider and Stoll[16] show that for a two-dimensional system with $\theta = 0.5$ the central peak in $S(q, \omega)$ appears at a temperature somewhere between 22% and 63% above the critical temperature. Our analysis predicts a displacive to order-disorder crossover at a temperature 30% above T_c and a central peak formation at that temperature. This seems to be in at least rough agreement with the molecular-dynamics results.

Let us reiterate that no long-range order appears at the crossover temperature, only a local ordering which causes a central peak to form in the dynamic response function.

V. CONCLUSION

We have developed an exact real-space renormalization-group technique for a continuous spin model in one dimension, based on the eigenvalues and eigenfunctions of the transfer operator for the system, and have applied it to the ϕ^4 model of structural phase transitions for the full range of the parameter space from the displacive limit to the Ising limit. We find that the critical universality class is clearly Ising-like. However, away from the critical fixed points the system displays two different kinds of noncritical RG flow, with a sharp crossover in between. One region of the parameter space flows to the Ising limit and another flows to a high-temperature fixed point associated with a system with a Gaussian-like symmetry. In this latter displacive region the dominant excitations of the system are anharmonic phonon oscillations about the center of the one-particle potential. Analysis of the RG flow in the crossover region well away from the fixed points leads us to the conclusion that the formation of domain walls drives the crossover from displacive to Ising-like behavior. In one dimension the crossover reduced temperature T_0 takes the form $T_0(\theta) \sim \theta^{3/2}$ for $\theta << 1$ (near the displacive limit).

A Kadanoff-Migdal transformation is used to produce an approximate RG for the two-dimensional ϕ^4 model. The Kadanoff-Migdal method is expected to give a reliable phase diagram in two dimensions. Our

conclusion is that the critical behavior remains strictly Ising-like in two dimensions; i.e., the system is in the same universality class as the Ising model. The crossover to displacive behavior still occurs near the displacive limit at a temperature $T_0(\theta) \approx 1.3 T_c(\theta)$. Above this temperature the primary excitations are anharmonic phonon oscillations about the high-symmetry points of the one-particle potential. For $T_c < T < T_0$ the primary excitations are mobile domain walls, the RG flow goes to the Ising limit and the crossover is driven by the domain-wall formation. The formation of oppositely ordered domains can be observed by the appearance of a peak at $\omega = 0$ in the dynamic response function $S(q, \omega)$ for q^{-1} less than the average domain size. At $T = T_c$ the system undergoes an Ising-like continuous transition into an ordered phase. Below T_c the dominant excitations are oscillations about the bottom of one side of the one-particle potential.

Presumably some of the techniques used here could be applied to block spin RG treatment of the two-dimensional ϕ^4 model.[17] If this is possible, a check on the capabilities of the Kadanoff-Migdal transformation for describing continuous spin systems could be obtained.

ACKNOWLEDGMENTS

We wish to acknowledge helpful discussions with Eytan Domany, Pierre Hohenberg, Alan Bishop, and Robert Guyer and a useful communication from Alistair Bruce. This work was supported by the U.S. Army Research Office under Grant No. DAAG-29-79-C-0097 and by the National Science Foundation through Grant No. DMR-76-81083A02 to the Cornell Materials Science Center.

---

*Present Address: Dept. of Phys., Rutgers Univ., Piscataway, N.J. 08854.

[1]R. A. Cowley, Adv. Phys. 29, 1 (1980); A. D. Bruce, *ibid.* 29, 111 (1980); A. D. Bruce and R. A. Cowley, *ibid.* 29, 219 (1980), and references therein.

[2]R. A. Cowley, Philos. Mag. 11, 673 (1964).

[3]J. A. Krumhansl and J. R. Schrieffer, Phys. Rev. B 11, 3535 (1975).

[4]T. Schneider and E. Stoll, Phys. Rev. B 13, 1216 (1976).

[5]K. G. Wilson and J. Kogut, Phys. Rep. 12C, 76 (1974).

[6]R. Morf, T. Schneider, and E. Stoll, Phys. Rev. B 16, 462 (1977).

[7]A. D. Bruce, T. Schneider, and E. Stoll, Phys. Rev. Lett. 43, 1284 (1979).

[8]T. Niemeijer and J. M. J. van Leeuwen, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 6, p. 425, and references therein.

[9]A. D. Bruce and T. Schneider, Phys. Rev. B 16, 3991 (1977).

[10]T. W. Burkhardt and W. Kinzel, Phys. Rev. B 20, 4730 (1979).

[11]L. Kadanoff, Ann. Phys. (N.Y.) 100, 359 (1976); A. A. Migdal, Zh. Eksp. Teor. Fiz. 69, 810, 1457 (1975) [Sov. Phys. JETP 42, 743 (1976)].

[12]D. R. Nelson and M. E. Fisher, Ann. Phys. (N.Y.) 91, 226 (1975).

[13]D. J. Scalapino, M. Sears, and R. S. Ferrell, Phys. Rev. B 6, 3409 (1975).

[14]R. Morf and H. Thomas, Z. Phys. B 23, 81 (1976).

[15]M. Abramowitz and Irene E. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965).

[16]T. Schneider and E. Stoll, in *Ferroelectrics,* edited by R. Blinc (Gordon and Breach, New York, 1980), Vol. 24, p. 67.