Critical and crossover behavior of the two-dimensional ϕ^4 model on a lattice

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A real-space renormalization-group transformation has been carried out on the classical ϕ^4 model on a lattice in two dimensions. The critical line has been found for $0 < \theta < \infty$ where θ is the ratio of the site well depth to the nearest-neighbor harmonic coupling energy. For $\theta << 1$ (near the displacive limit) the critical temperature qualitatively agrees with a rigorously derived function for $T_c(\theta)$ in that limit. In contrast, a previously published Kadanoff-Migdal transformation on the same model predicts that $T_c(\theta)$ is linear in θ for $\theta << 1$. A crossover to noncritical Gaussian-like behavior is found at temperature $T_0(\theta) > T_c(\theta)$ for sufficiently small θ.

I. INTRODUCTION

The ϕ^4 model on a lattice is defined by the reduced Hamiltonian

$$\frac{H}{k_B T} = K \sum_i \frac{p_i^2}{2m} + \sum_i U_1(x_i) + \sum_{(ij)} U_2(x_i,x_j) \quad , \tag{1a}$$

$$U_1(x) = \frac{-K\theta}{2}x^2 + \frac{K(\theta+1)}{4}x^4 \quad , \tag{1b}$$

$$U_2(x,y) = \frac{K}{2}(x-y)^2 \quad , \tag{1c}$$

where $K = 1/k_B T$, $\{x_i\}$, and $\{p_i\}$ are coordinates and momenta of the particles and (ij) are nearest-neighbor pairs. θ is proportional to the ratio of the well depth of the site potential energy to the harmonic strain energy. In the limit $\theta \rightarrow \infty$ the ϕ^4 model is formally equivalent to the Ising model. The limit $\theta \rightarrow 0$ is called the displacive limit. In that limit the well depth of U_1 is zero. U_1 has only a single minimum and so the Hamiltonian has a Gaussian-like[1] structure in that limit. In d dimensions, the canonical configurational partition function is defined by

$$Q_N(K,\theta) = \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_N \prod_{(ij)} e^{G(x_i,x_j)} \quad , \tag{2a}$$

A real-space renormalization-group (RG) transformation can be performed in two dimensions by integrating over half the coordinates in a way similar to the decimation procedures that have been used on the two-dimensional Ising model.[2] Block-spin RG's on ϕ^4 type models have also been constructed.[3] I have found by a numerical integration technique that for most of the (K,θ) parameter space the renormalized couplings can be accurately mapped onto the ϕ^4 Hamiltonian without introducing further couplings. The only exception is in the low-temperature region near the Ising limit. Examination of the RG flow along the critical manifold $T_c(\theta)$ indicates that θ is a marginal parameter near the Ising critical fixed point. For very large θ the renormalized value of θ is found to be larger by only a small additive constant. This is an artifact of the decimation character of the RG transformation and therefore probably has no effect on the Ising universality of the phase transition. For $\theta << 1$, near the displacive limit where the well depth of U_1 is small, the critical temperature is not proportional to the harmonic strain energy as is the case in three or higher dimensions.[4] However this numerical solution to $T_c(\theta)$ is in qualitative agreement with a rigorous formula for the critical temperature near the displacive limit derived by Bricmont and Fontaine.[5] They show that $T_c(\theta)$ is bounded above and below by a function of the form

$$\theta = -C(\theta+1)T\ln[(\theta+1)T] \tag{3}$$

near the displacive limit. A Kadanoff-Migdal transformation[6] on the same model[7] in two dimensions predicts that T_c is linear in θ for small θ. In general the Kadanoff-Migdal transformation predicts $T_c \sim \theta^{2-d/2}$ in d dimensions for small θ. Not surprisingly the Kadanoff-Migdal transformation simply misses the logarithmic correction to the linear behavior in two dimensions.

The existence of a crossover from Gaussian-like to Ising-like behavior at small θ predicted by the Kadanoff-Migdal transformation[7] is confirmed by this RG transformation. For T greater that a crossover temperature $T_0(\theta)$ the system exhibits a Gaussian-like symmetry after the RG transformation has been iterated several times. This means that the double well potential is renormalized into a single well potential similar to the Gaussian model.[1] As T is lowered this behavior disappears and the system crosses over to an Ising-like potential in which the well depth increases after each iteration of the RG transformation. In this region small blocks of particles would tend to have a nonzero net polarization. This crossover should be associated with the emergence of a central peak in the dynamic response function $S(q,\omega)$.[7]

II. RESULTS AND DISCUSSION

The RG transformation applied here is very similar in principle to RG transformations used on the Ising model in two dimensions.[2] Figure 1(a) shows a square lattice in two dimensions. The bonds represent the pair couplings $G(x,y)$. The first step is to integrate Eq. (2) over the sites marked $\times$. The remaining sites form a square lattice with nearest-neighbor distance $\sqrt{2}$ times the original nearest-neighbor distance. If it now proves possible to map the new effective couplings between the remaining lattice sites onto the ϕ^4 Hamiltonian then a RG transformation with scale change $b=\sqrt{2}$ can be generated. When the variable labeled t in Fig. 1(a) is integrated over, a coupling symmetric in (x_1,x_2,x_3,x_4) is generated:

$$\exp[\tilde{G}_4(x_1,x_2,x_3,x_4)] = \int_{-\infty}^{\infty} dt \exp[G(x_1,t)+G(x_2,t)+G(x_3,t)+G(x_4,t)] \quad . \tag{4}$$

$\tilde{G}_4$ is invariant under permutation of any two of its arguments. Therefore the integration creates equally strong couplings between nearest neighbors and next nearest neighbors. In addition, each nearest-neighbor bond will have a contribution coming from another integral. One can approximate the effect of the next-nearest-neighbor couplings by adding their strength to the nearest-neighbor couplings.[2] In the Ising limit this procedure gives both the critical temperature and exponents quite accurately.[2] If this procedure is to make any sense in the general case then the following equation must be approximately satisfied:

$$\tilde{G}_4(x_1,x_2,x_3,x_4) = \frac{-1}{4}\sum_{i=1}^{4}\tilde{U}_1(x_i) - \tfrac{1}{2}[\tilde{U}_2(x_1,x_2)+\tilde{U}_2(x_2,x_3)+\tilde{U}_2(x_3,x_4)+\tilde{U}_2(x_4,x_1)] \quad , \tag{5}$$

where

$$\tilde{U}_1(x) = -\tilde{G}_4(x,x,x,x) \quad , \tag{6}$$

i.e., the renormalized couplings can be approximately split into site terms and couplings between nearest neighbors only. $\tilde{U}_1$ is the site potential term and $\tilde{U}_2$ is the effective nearest-neighbor coupling. This procedure is carried out by numerically integrating Eq. (4) and performing the steps listed below numerically. The function $\tilde{U}_1(x)$ is very accurately fit over the entire parameter space by the ϕ^4 site potential term

$$\frac{-\tilde{K}\tilde{\theta}}{2}\left(\frac{x}{\tilde{\zeta}}\right)^2 + \frac{\tilde{K}(\tilde{\theta}+1)}{4}\left(\frac{x}{\tilde{\zeta}}\right)^4 \quad .$$

$\tilde{K}$ and $\tilde{\theta}$ are the renormalized coupling constants and $\tilde{\zeta}$ is a site length rescaling factor. Once $\tilde{U}_1$ is known, the minima of the function are located numerically. For most of the parameter space $\tilde{U}_1$ has two minima located at $\pm x_0$. The strain energy between nearby sites is measured by letting the arguments in $\tilde{G}_4$ take on different values. For example, I define the functions

$$\tilde{U}_2^{(1)}(x_0,y) = -\tilde{G}_4(x_0,x_0,x_0,y) - \tfrac{3}{4}\tilde{U}_1(x_0) - \tfrac{1}{4}\tilde{U}_1(y) \quad , \tag{7a}$$

$$\tilde{U}_2^{(2)}(x_0,y) = -\tfrac{3}{4}[\tilde{G}_4(x_0,x_0,y,y) + \tfrac{1}{2}\tilde{U}_1(x_0) + \tfrac{1}{2}\tilde{U}_1(y)] \quad . \tag{7b}$$

The first corresponds to fixing three particles in the block in Fig. 1(b) at x_0 and displacing the fourth to y. The second corresponds to fixing two at x_0 and displacing two to y. Of course other combinations are possible but these are representative; if these two functions are nearly equal then this method of dividing up $\tilde{G}_4$ is reasonable. The difference between these two functions is a measure of the error made in assuming nearest-neighbor couplings only. Every-

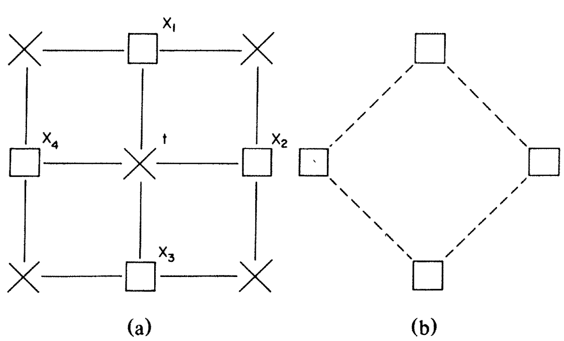

FIG. 1. The first step of the RG procedure consists of integrating $\exp(-H/k_BT)$ over the lattice sites marked $\times$ in Fig. 1(a). Figure (b) shows that the sites that remain also form a square lattice, but with the lattice constant increased by a factor of $\sqrt{2}$.

where in the parameter space except at low temperature near the Ising limit these two functions are very close to being equal. For example, the case of $\theta = 10$ and T on the critical line is shown in Fig. 2. All other cases except the low-temperature Ising region give similar agreement. Even there the two functions differ by only about 50%. Once $\tilde{U}_1$ and $\tilde{U}_2^{(2)}$ are determined, the renormalized coupling constants $\tilde{K}$ and $\tilde{\theta}$ are determined from

$$\frac{\tilde{K}\tilde{\theta}^2}{4(\tilde{\theta}+1)} = -[\tilde{U}_1(x_0) - \tilde{U}_1(0)] \ , \tag{8a}$$

$$\frac{2\tilde{K}\tilde{\theta}}{\tilde{\theta}+1} = \tilde{U}_2^{(2)}(x_0, -x_0) \ . \tag{8b}$$

These equations are chosen so that the four point coupling function $\tilde{G}_4(x_1,x_2,x_3;x_4)$ is fit exactly by the ϕ^4 Hamiltonian at the points $(0,0,0,0)$, (x_0,x_0,x_0,x_0), and $(x_0,x_0,-x_0,-x_0)$. Alternatively one can parametrize the renormalized potential by the width of the double well rather than the height. This could be important near the Ising limit because the particles seldom sample the potential near the top of the well. It turns out that the RG flow with that parametrization is almost identical to the first parametrization. This in addition to the careful checking of the difference between $U_2^{(1)}$ and $U_2^{(2)}$ and a comparison with an asymptotic expansion of Eq. (4) near the Ising limit assures that this scheme is reasonable.

The RG flow of the system has the following features as shown in Figs. 3(a) and 3(b). The RG flow is determined by performing the above steps numerically and iterating. The critical manifold $T_c(\theta)$ extends from $\theta = 0$, to $\theta = \infty$. Near $\theta = 0$, $T_c(\theta)$ tends to zero slightly faster than the first power of θ, i.e., T_c is not proportional to the nearest-neighbor strain energy as it is in higher dimensions.[4] In some recent work, Bricmont and Fontaine[5] have shown

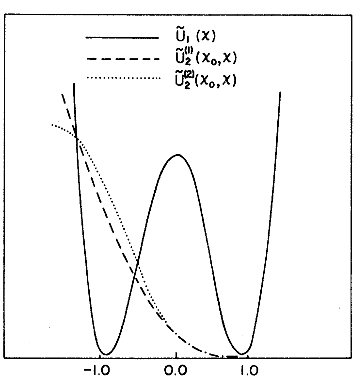

FIG. 2. The shape of the renormalized potentials on the critical line near the Ising limit ($T = 0.95$, $\theta = 10.0$). The vertical scales for the one particle and two particle potentials are vastly different. x_0 is the point where $\tilde{U}_1$ takes its minimum value.

that for $\theta << 1$ the critical temperature is bounded above and below by a function of the form

$$\theta = -C(\theta+1)T\ln[(\theta+1)T] \ . \tag{9}$$

This was accomplished by using a Peierls argument. The lower bound was found by using an infrared bound technique and the upper bound was found by using correlation inequalities. Since the critical temperature is bounded above and below by a function of this form it is reasonable to assume that $T_c(\theta)$ obeys the relation

$$\theta \approx -C(\theta+1)T_c\ln[(\theta+1)T_c] \tag{10}$$

for some C as $\theta \to 0$. In addition Bricmont and Fontaine conjecture without proof that $C = 3/4\pi$. This agrees qualitatively with the results of this RG analysis. Figure 3(b) compares a curve of the form (10) (solid line) with the points on the critical line given by the RG flow (circles). The constant C is chosen so that the curve goes through the value of T_c at $\theta = 0.08$. This constant is about five times bigger than the conjecture of Bricmont and Fontaine.

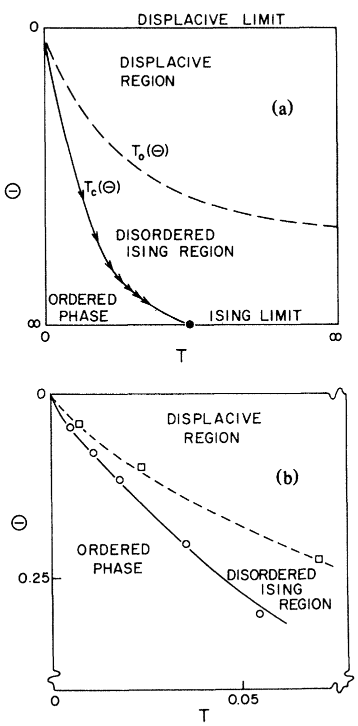

FIG. 3. The phase diagram of the ϕ^4 model in two dimensions. Figure (a) shows the entire parameter space. Figure (b) is an enlargement of the top left corner of (a). The circles are points on the critical line as determined by the RG analysis. The solid line is the prediction of Bricmont and Fontaine with the constant C chosen so that the line passes through the left-most point. The squares and dotted line are the corresponding point on the crossover line. The arrows denote the RG flow along the critical manifold.

Also shown are points on the crossover line (squares) fit with Eq. (10). The Kadanoff-Migdal transformation[7] gives a straight line which lies far above the curves shown here. Near the Ising limit I find that the critical temperature obeys the relation $T_c(\theta) \approx T_c(\infty) - \mathrm{const}/\theta$.

Some recent work by Baker and Bishop[8] on an exactly solvable model in this universality class is in qualitative agreement with this phase diagram. Their parametrization is somewhat different from this work but the essential division of the phase diagram into an ordered phase, a disordered Ising-like region and a Gaussian-like region is preserved.

III. CONCLUSION

In conclusion, I have used a real-space RG procedure to determine the phase diagram of the ϕ^4 model in two dimensions. Near the displacive limit the critical temperature agrees qualitatively with a rigorous formula for T_c in that limit. A Kadanoff-Migdal transformation[7] was incorrect in this respect. However, the Kadanoff-Migdal transformation does correctly predict the existence of a high-temperature Gaussian-like region for sufficiently small θ.

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