Transitions and modulated phases in centrosymmetric ferroelectrics: Mean-field and renormalization-group predictions

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A variety of ferrodisplacive transitions have Landau expansions which involve terms proportional to $p^2(\partial p)$, i.e., three powers of the order parameter (p) and one gradient (∂). Such expansions have also been suggested for polymeric liquid crystals. We have studied a rotationally invariant, centrosymmetric ferroelectric in which the order parameter is a vector. The $p^2\partial p$ term leads to modulated phases when it is large enough. The modulated phase close to the uniform-modulated transition and the location of the transition are discussed as a function of dimensionless parameters in a simple model for the free energy. Modifications expected from dangerous irrelevant variables are discussed. The free energy is studied within the $d=4-\epsilon$ renormalization group. A number of fixed points (always including a stable fixed point) are found as a function of the number of components of the order parameter and the dimensionality of space. The fixed points and the renormalization-group flows are discussed. Finally, the nature of the transition when both mean-field theory and the renormalization group are taken into account is discussed.

I. INTRODUCTION

Since the discovery of the renormalization group[1] our understanding of the behavior of a variety of systems near phase transitions has greatly increased. However, relatively little work has been done on systems[2–9] which allow, in the Landau expansion,[10] terms proportional to $p^2(\partial p)$, i.e., to three powers of the order parameter (p) and one gradient (∂). Such systems seem to have been studied relatively little even within the mean-field approximation. As a variety of ferrodisplacive transitions and certain liquid-crystal[11–14] transitions allow such terms, their study is of considerable interest. It has also been suggested[15] that free energies of this nature are relevant to certain polymeric systems.

In this paper we will discuss a simple, mathematically (relatively) tractable example of such a transition; a system in which the order parameter is an n-component vector in d dimensions with $n \neq d$ (but $n \leq d$), which is odd under spatial inversion and even under time reversal. In general, such an order parameter is expected to couple linearly to the electric field. In consequence, long-range interactions may be expected for the order parameter. We will assume that this long-range interaction can be ignored, either because the coupling to the electric field is small or because the long-range interactions are screened by charged impurities. This simple model has only three essential parameters and is in consequence substantially easier to treat than models of more realistic systems. In addition the model for $n=d=2$ describes chiral smectic C, F, or I films and, more generally, for $n=2$, $d=3$ chiral smectic C, F, or I systems in which the pitch of the director helix is very large. Thus this model is both a mathematically simple prototype for an interesting class of phase transitions and a physically relevant model.

This paper is organized as follows. In the next section we give the Landau expansion for this system and analyze it within mean-field theory. The interactions between the $(\partial p)^2$, $p^2\partial p$, and p^4 terms in a simple Landau expansion lead to interesting transitions between uniform and modulated phases which are second order (in less than four spatial dimensions) although this is not the prediction of a simple Landau analysis and, even within mean-field theory, have thermodynamic derivatives which diverge with dimension-dependent exponents. Near the uniform-modulated phase boundary the modulated phase has a very slow modulation and is not well described by a small number of spatial harmonics of the order parameter, and must be treated by nonstandard methods. However, we find that the order parameter is not large in the modulated phase and that, except near the uniform-modulated phase boundary, the modulated phase *is* well described by a small number of spatial harmonics of the order parameter. It is also shown that our description of the uniform-modulated phase transition must be modified very near the transition due to the presence of "dangerous" irrelevant variables.

Sec. III discusses the renormalization-group treatment of this system. In contrast to previous work,[7] we find that there are a number of fixed points including a stable fixed point for $d=4-\epsilon$ and all n, $d \geq n \geq 2$. For certain ranges of n and d the flow near these fixed points is helical, i.e., is characterized by complex eigenvalues. The stability of the fixed points is discussed, as are the gross renormalization group flows.

Finally, in the last section we discuss our results and the behavior expected in actual fluctuating systems from the combination of the mean-field and renormalization-group results.

II. MEAN-FIELD THEORY

In this section we will discuss the phase-transition behavior of centrosymmetric ferroelectrics without long-range interactions at the level of Landau mean-field theory. That is, we will assume that the order parameter (the polarization $\mathbf{p}$) is small in magnitude and slowly varying so that the free energy can be expanded in powers of $\mathbf{p}$ and the gradients. We then discuss the nature of the minimum of this free energy as a function of the parameters which appear in this expansion.

We will write the free-energy functional (FEF) as

$$F=\sum_{m} F_{2m} , \tag{2.1}$$

where

$$F_2=\int d\mathbf{X}\tfrac{1}{2}r \mid \mathbf{p}\mid^2 , \tag{2.2}$$

and

$$F_4=\int d\mathbf{X}\{\tfrac{1}{2}[(1-\Delta)\mid \nabla\cdot\mathbf{p}\mid^2+(1+\Delta)\mid \nabla\times\mathbf{p}\mid^2 + \mid \nabla_N\mathbf{p}\mid^2]+w \mid \mathbf{p}\mid^2\nabla\cdot\mathbf{p}+u \mid \mathbf{p}\mid^4\} . \tag{2.3}$$

We have not displayed the F_{2m} explicitly for $m>2$ (they are rather complex). Here $\mathbf{p}$ is an n-component-vector order parameter in d-dimensional space $\mathbf{X}\equiv(\mathbf{x},\mathbf{x}_N)$ with $n\le d$. The coordinates of the n components of $\mathbf{X}$ in the space spanned by $\mathbf{p}$ are given by $\mathbf{x}$ and the remaining $d-n$ components normal to any $\mathbf{p}$ are given by $\mathbf{x}_N$, ∇ is a gradient in the n-dimensional space of $\mathbf{p}$, and ∇_N is the gradient in the $(d-n)$-dimensional space normal to $\mathbf{p}$. The n directions in the subspace of $\mathbf{p}$ will be indexed by $\alpha=1,\ldots,n$ and the remainder by $\alpha=n+1,\ldots,d$. In general F_m would be the integral of the sum of arbitrary parameters multiplying all symmetry allowed terms containing $2\le m'<m$ powers of $\mathbf{p}$ and $m-m'$ powers of gradients. However, we will not be concerned in this paper with F_{2m} for $m>2$, except for certain qualitative features thereof. We will be primarily concerned with $\bar{F}=F_2+F_4$. In a region of interest, sufficiently close to the phase transition, the $\mathbf{p}(\mathbf{X})$ which minimizes $\bar{F}$ is (as will be shown below) small and slowly varying. Therefore the effect of the higher-order F's is expected to be small (but see Sec. II D below). The dimensions of $\mathbf{p}$ and $\mathbf{X}$ have been chosen so that $\nabla\mathbf{p}$ is dimensionless and $\mathbf{x}$ and $\mathbf{x}_N$ have been scaled differently so that the gradient terms in F_4 have the dimensionless form given above. We assume that the coefficients of all the $(\partial p)^2$ terms are non-negative so that this is possible. This implies that $-1\le\Delta\le1$ (i.e., the terms proportional to $1\pm\Delta$ cost energy). If this condition does not hold, Lifschitz transitions driven by the negative square gradient terms, are expected.

Now suppose $\mathbf{p}(\mathbf{X})$ is an arbitrary (but infinitely differentiable) function of $\mathbf{X}$ which does not tend to zero as $\mathbf{X}$ tends to infinity in any direction. Then if we make the transformation $\mathbf{p}(\mathbf{X})\to\lambda\mathbf{p}(\mathbf{X}\lambda)$ then $F_m\to\lambda^m F_m$. More generally if $\mathbf{p}\to0$ sufficiently rapidly as $\mathbf{X}\to\infty$ in D dimensions so that there are no contributions to the free energy as $\mathbf{X}\to\infty$ in those dimensions, then $F_m\to\lambda^{m-D}F_m$ under this transformation. It follows that either F_m is bounded below by zero or it is not bounded below. Throughout this paper we will assume that F_m is bounded below for $m>4$ and, in fact, that $F_m=0$ only if $\mathbf{p}(\mathbf{X})$ is identically zero for all values of $\mathbf{X}$. If F_m is not bounded below for $m>4$ then there will generally be first-order transitions which preempt the transitions discussed below.

If the F_m for $m>4$ are bounded from below it follows that the disordered state $\mathbf{p}=\mathbf{0}$ is the minimum free-energy state when F_2 and F_4 are both bounded below. Provided F_4 is bounded below there will be a transition from this disordered state to an ordered state when F_2 stops being bounded from below ($r=0$). This ordered state may be either a uniform state ($\mathbf{p}$ constant) or a modulated state ($\mathbf{p}$ not constant) depending on dimensionless combinations of the parameters in F_4. There are two such dimensionless parameters in F_4 which we will parametrize by Δ and $1+\zeta=2(1-\Delta)uw^{-2}$. There may be a transition from the uniform state to a modulated state along some surface in this parameter space described by a function $\zeta_u(\Delta)$. Along some (possibly different) surface, $\zeta_t(\Delta)$, F_4 will cease to be bounded from below.

A. Bounds on the free energy

It can be shown that for $\zeta>\zeta_t$ there is a second-order transition ($f=\bar{F}/V\sim r^2$, where V is the volume) from a disordered ($\mathbf{p}=\mathbf{0}$) state to an ordered state when $r=0$. Suppose M is the value of p for the uniform state which minimizes the free energy $\bar{F}$. We easily see that $M=0$ for $r>0$, $M^2=\mid r\mid/(4u)$ for $r<0$, and $f_u=\bar{F}V^{-1}$ in the uniform state where $f_u=-\frac{1}{4}\mid r\mid M^2$. We see that for $\zeta>\zeta_t$

$$\tfrac{1}{2}r\langle p^2\rangle+(\zeta-\zeta_t)u\langle p^2\rangle^2 \le\tfrac{1}{2}\langle p^2\rangle+(\zeta-\zeta_t)u\langle p^4\rangle\le f\le f_u , \tag{2.4}$$

where $\langle p^m\rangle=V^{-1}\int d\mathbf{X}\mid\mathbf{p}(\mathbf{X})\mid^m$. The first inequality follows from the Schwartz inequality, the second from the definition of ζ_t, and the last because the absolute minimum of the free energy is bounded above by the (constrained) uniform minimum. Clearly therefore $-(\zeta-\zeta_t)^{-1}\le\mid f_u\mid^{-1}f\le-1$. It is also clear that the order-disorder transition is first order for $\zeta<\zeta_t$. In particular, consider any state $\mathbf{p}(\mathbf{X})$ which (a) does not tend to zero in any direction as $X\to\infty$ in any direction and (b) has $F_4(\mathbf{p})$ negative. A state satisfying (b) exists by definition when $\zeta<\zeta_t$. States satisfying (a) and (b) can be constructed from states which satisfy only (b), as shall be shown below. The free energy for the state $\lambda\mathbf{p}(\mathbf{X}\lambda)$ is, for small enough λ,

$$F=\tfrac{1}{2}rV\langle p^2\rangle\lambda^2+F_4(p)\lambda^4+F_6(p)\lambda^6+O(\lambda^8) . \tag{2.5}$$

Now $F_4(p)$ is negative by construction and $\langle p^2\rangle$ and $F_6(p)$ are positive by construction. For a range of positive r, $0<r<[F_4(p)]^2[2F_6(p)V\langle p^2\rangle]^{-1}$, this formula for F is negative for a range of λ^2. As $r\to0$ this range of λ^2

includes arbitrarily small λ. Thus the minimum of the free energy is negative for sufficiently small positive r. However, for any positive r there are no states with negative free energy arbitrarily close to the disordered state. Thus the transition must be a first-order transition at some positive r to an ordered state with $\langle p^2\rangle=\partial f/\partial r \neq 0$.

It is possible to show that F_4 is bounded from below and that the uniform state is the absolute minimum provided $\zeta>0$. We can write

$$\bar{F}=\int d\mathbf{X}\left\{\frac{1}{2}\left[(1-\Delta)\left[\nabla\cdot\mathbf{p}+\frac{w}{(1-\Delta)}(|\mathbf{p}|^2-M^2)\right]^2+(1+\Delta)|\nabla\times\mathbf{p}|^2+|\nabla_N\mathbf{p}|^2\right]+\zeta\frac{w^2}{2(1-\Delta)}(|\mathbf{p}|^2-M^2)^2+f_u\right\}. \quad (2.6)$$

As all the p-dependent terms in Eq. (2.6) are clearly positive for $\zeta>0$ it follows that $\zeta_u(\Delta)<0$ and $\zeta_t(\Delta)<0$. It is also easy to see that $\zeta_u(\Delta)>0$ as the uniform state[8] is linearly unstable for $\zeta<0$ so that $\zeta_u(\Delta)=0$.

It is not so easy to calculate ζ_t for arbitrary n, although it is possible to bound it. For this purpose we write F_4

$$F_4=\int d\mathbf{X}\tfrac{1}{2}\left[(1-\Delta)\left[\nabla\cdot\mathbf{p}+\frac{w}{(1-\Delta)}|\mathbf{p}|^2\right]^2+(1+\Delta)|\nabla\times\mathbf{p}|^2+|\nabla_N\mathbf{p}|^2+\zeta\frac{w^2}{(1-\Delta)}|\mathbf{p}|^4\right]. \quad (2.7)$$

It is clear that if any p has F_4 negative then a $\mathbf{p}$ which depends only on $\mathbf{x}$ (the n components of $\mathbf{p}$) will also have F_4 negative. In consequence we restrict our attention to $\mathbf{p}$'s which have this property. If we additionally restrict our attention to $\mathbf{p}$'s which have zero curl ($\nabla\times\mathbf{p}=0$) we will find an upper bound for ζ_t and $\mathbf{p}$ can be written as the gradient of a potential. If we write[16] $\mathbf{p}=(1-\Delta)w^{-1}\nabla\ln(\psi)$ we find the remarkable simplification

$$F_4=\tfrac{1}{2}(1-\Delta)^3w^{-2}V_N\int d\mathbf{x}[(\psi^{-1}\nabla^2\psi)^2+\zeta|\psi^{-1}\nabla\psi|^4] \quad (2.8)$$

where $V_N=\int d^{d-n}x_N$ is the volume of the space normal to $\mathbf{p}$. For a simple variational calculation the Laplacian of ψ can be chosen to be

$$\nabla^2\psi=\begin{cases}0 & (x>a)\,,\\ \dfrac{qn}{a^nS_n} & (x\le a)\,,\end{cases} \quad (2.9)$$

where $S_n=2\pi^{n/2}/\Gamma(n/2)$ is the surface area of the n-dimensional unit sphere. The solution of (2.9) is

$$\psi(x)=\begin{cases}\dfrac{qx^{2-n}}{(n-2)}S_n^{-1} & (x>a)\,,\\ \dfrac{qa^{-n}}{2}S_n^{-1}\left[\dfrac{a^2n}{(n-2)}-x^2\right] & (x\le a)\,.\end{cases} \quad (2.10)$$

The free energy (2.8) was then calculated to leading order in $\bar{\epsilon}=4-n$ by integrating inside the spherical radius from $0\le x\le a$ and outside the sphere from $a<x<\infty$. The integral of (2.8) is zero for $x>a$ because there is no charge outside $x=a$. For $x<a$ it is given by

$$\int dx\,x^{n-1}(\psi^{-1}\nabla^2\psi)=4(\tfrac{1}{2}a)^{-\bar{\epsilon}}[\tfrac{4}{3}-\ln(2)]\,. \quad (2.11)$$

The integral of the quartic term will be calculated explicitly for $x>a$, yielding

$$\zeta\int dx\,(\psi^{-1}\nabla\psi)^4x^{n-1}=\zeta(2-\bar{\epsilon})^4\int_a^\infty x^{n-5}dx=\zeta(2-\bar{\epsilon})^4\frac{a^{-\bar{\epsilon}}}{\bar{\epsilon}}\,. \quad (2.12)$$

The integral of the quartic term inside $x=a$ yields integrals similar to (2.11). However, these contributions are all of order one so the leading term is the $1/\bar{\epsilon}$ term of (2.12). Thus the free energy diverges to $-\infty$ as $\bar{\epsilon}\to 0$ and $a\to 0$ if $\zeta<0$. Therefore we have the condition that $\zeta>0$ or $w^2/[2u(1-\Delta)]<1$ for F_4 to be bounded from below for $n=4$. It follows, therefore, that $\zeta_t=0$ provided $n=4$.

Note that while $\mathbf{p}$ for the state considered above goes to zero in all directions it is easy to construct states which have negative F_4 and do not go to zero in any direction as $\mathbf{x}$ goes to infinity. This can be done simply by placing equal charges in small hyperspheres around the points of an infinite, n-dimensional lattice. When the radius of these hyperspheres is much less than the lattice spacing and ζ is negative, F_4 will be negative. However, for $n<4$, $\zeta=0$, F_4 will be zero only if $\nabla^2\psi=0$ everywhere but ψ is never infinite or zero, as the discussion above shows that the divergence in p implied by zeros or infinities of ψ has infinite free energy. We therefore expect that $\zeta_t<0$, and, in fact, prove this below.

First, however, we will give an upper bound for ζ_t for $n<4$. This will be done by assuming that

$$\mathbf{p}=(1-\Delta)w^{-1}\hat{\mathbf{x}}g(|x|)/|x|\,.$$

The free energy (2.7) then becomes

$$\bar{F}=\frac{(1-\Delta)^3}{2w^2}V_NS_n\int dx\left\{x^{n-5}[(n-2)g^2+2(n-2)g^3+g^4(1+\zeta)]+x^{n-4}[2(n-2)g+2g^2]\frac{dg}{dx}+x^{n-3}\left[\left[\frac{dg}{dx}\right]^2-g^2\right]\right\}. \quad (2.13)$$

The following procedure was then used to write $\tilde{F}$ in convenient form; (i) the term proportional to x^{n-4} was integrated by parts, (ii) the substitution $z=\ln x$ was made, and (iii) n was replaced by $4-\bar{\epsilon}$. The result is

$$\tilde{F}=\frac{(1-\Delta)^3}{2w^2}V_N S_n \int dz\, e^{-\bar{\epsilon}z}[V(g)+g'^2]\ , \qquad (2.14)$$

where

$$V(g)=2(2-\bar{\epsilon})g^2+4(1-\bar{\epsilon}/3)g^3+(1+\zeta)g^4\ ,$$

$g'=dg/dz$. Since the integrand of $\tilde{F}$ is proportional to $V(g)+g'^2$, $\tilde{F}$ can be less than zero only if $V(g)$ has enough negative contributions. Therefore the function $V(g)$ was minimized by taking $dV/dg=0$ yielding $g_{\min}$. A minimum value for the ζ for which $\tilde{F}$ is negative is that value which $V(g_{\min})=0$. This minimum value of ζ is found to be

$$1+\zeta=2(1-\bar{\epsilon})/3)/(2-\bar{\epsilon})\ .$$

For $n=3$ ($\bar{\epsilon}=1$), $\zeta<-\frac{1}{9}$. For $n=2$ ($\bar{\epsilon}=2$) $\zeta<-1$, that is, no useful lower bound on ζ_t results. Although this lower bound for the upper bound on ζ was found analytically, the actual value of ζ_t for which $\tilde{F}$ is negative must be determined numerically. This was accomplished by means of a variational calculation, replacing g with $g+\delta g$ and expanding $\tilde{F}$ and setting the term of first order in δg equal to zero, yielding

$$2(2-\bar{\epsilon})g+(6-2\bar{\epsilon})g^2+2(1+\zeta)g^3+\bar{\epsilon}g'-g''=0\ . \qquad (2.15)$$

However, as we have shown above, there is no nonzero minimum for $\tilde{F}$, essentially because a change in length scale will change the free energy. Thus, to find a minimum of $\tilde{F}$ we must specify a length scale. This is done most easily by insisting that $g=0$ for some (specified) value of $z=z_0$ [it is easy to see from the form of Eq. (2.15) that all solutions, except those with (positive) infinite free energy are zero at some (unspecified) value of z]. At z_0 no variation in g is allowed so that Eq. (2.15) need not be satisfied at z_0. It is then easy to show that the function g which minimizes $\tilde{F}$ subject to $g(z_0)=0$ is identically zero for $z<z_0$ and that $g\to g_{\min}$ as $z\to\infty$.

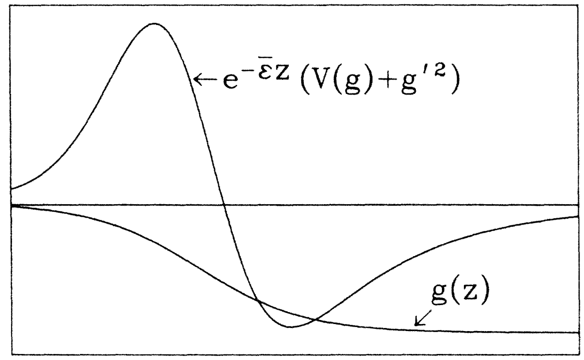

FIG. 1. Plot of the function $e^{-\bar{\epsilon}z}(V(g)+g'^2)$ with the numerical solution $g(z)$ for $\bar{\epsilon}=1$ and $\zeta=-0.37$.

The differential equation was solved numerically and the free energy was integrated numerically to determine the largest ζ for which $\tilde{F}$ is negative. The solution $g(z)$ of Eq. (2.15) was calculated starting at $z=0$, $g=g_{\min}$, and a small negative slope g'. Two behaviors for g were found. For $|\zeta|$ too small g diverged. For sufficiently large and negative ζ, g was zero at some z which (*a posteriori*) was chosen to be z_0 and the integration was stopped. The least negative value for ζ for which $\tilde{F}$ was found to be negative for $n=3$ is $\zeta_t\geq-0.37$. The previous upper bound for ζ_t given by Blankschtein *et al.*, using a trial function with a small number of spatial harmonics, was[8] $\zeta_t=-\frac{15}{19}=-0.79$. For $\zeta_t=-0.37$ the free energy is found to be small and negative in the interval integrating from $z=\infty$ to about $z\simeq-5.5$. For ζ less than but close to -0.37, $g(z)$ tends slowly to zero (see Fig. 1). In this region the overall free energy is positive. For $\zeta\lesssim-0.37$ $g(z)$ approaches zero but never reaches it and eventually diverges to $-\infty$.

It is also possible to give lower bounds for ζ_t. In particular for $\Delta>0$ we can write

$$F_4=\int d\mathbf{X}\left[\frac{1}{2}\left[2\Delta|\nabla\times\mathbf{p}|^2+|\nabla_N\mathbf{p}|^2+(1-\Delta)\sum_{i,j}(\partial_i p_j+sp_ip_j+s'\delta_{ij}|\mathbf{p}|^2)^2\right]+u'(s,s')|\mathbf{p}|^4\right]\ , \qquad (2.16)$$

provided $w=(1-\Delta)(s'-s/2)$ and

$$u'(s,s')=u-\tfrac{1}{2}(1-\Delta)(s^2+2ss'+ns'^2)\ .$$

We have used the identity

$$\int d\mathbf{X}\, p_ip_j\partial_ip_j=-\frac{1}{2}\int d\mathbf{X}\, p_j^2\partial_ip_i\ , \qquad (2.17)$$

which follows from integration by parts. Now provided $u'>0$, all terms in this equation are obviously positive. Thus we can find a bound on ζ_t by maximizing u' with respect to s using the relationship between s and s' from the formula for w. We find

$$u'\leq u-2(n-1)w^2/[(1-\Delta)(n+8)]\ .$$

Thus u can be chosen to be positive provided $1+\zeta>4(n-1)/(n+8)$ so that $1+\zeta_t<4(n-1)/(n+8)$.

Similarly for $\Delta<0$ we can write

$$F_4=\int d\mathbf{X}\left[\frac{1}{2}\left[-2\Delta(\nabla\cdot\mathbf{p}+s''\mathbf{p}^2)^2+|\nabla_N\mathbf{p}|^2+(1+\Delta)\sum_{i,j}(\partial_ip_j+sp_ip_j+s'\delta_{ij}|\mathbf{p}|^2)^2\right.\right.$$
$$\left.\left.+u''(s,s',s'')|\mathbf{p}|^4\right]\right]\ , \qquad (2.18)$$

provided

$$w=-2\Delta s''+(1+\Delta)(s'-s/2)$$

and

$$u''(s,s',s'')=u-\tfrac{1}{2}(1+\Delta)(s^2+2ss'+ns'^2)+\Delta s''^2 .$$

Again all terms are obviously positive so by maximizing u'' we find a bound on ζ_t;

$$1+\zeta_t<4(n-1)(1-\Delta)/[(n+8)(1+\Delta)-8(n-1)\Delta] .$$

It follows that for all Δ, $n<4$, there is a finite region in which there is a second-order transition to a spatially varying phase within mean-field theory. For $n=3$ and $\Delta>0$, ζ_t is bounded from above and below by $-0.27>\zeta_t>-0.37$. For $n=2$, $\Delta=0$, Felix *et al.*[9] have shown that $\zeta_t<-\frac{5}{9}$, which agrees with the value obtained from Eq. (2.16) for $\Delta\geq 0$. A lower bound $\zeta_t\geq -0.83$ for $n=2$, has been calculated by Blanckstein *et al.*[8] using a trial function with a small number of spatial harmonics. Thus we have shown that for $n<4$, ζ_t is nonzero and have bounded it from above and below.

B. Modulated state: Proof of finiteness and smoothness

We now discuss the nature of the minimum of the free-energy functional equation (2.6) when $0=\zeta_u>\zeta>\zeta_t$. It is expected[9] that the function $\mathbf{p}(\mathbf{x})$ which minimizes $\bar{F}$ in the modulated state can not be precisely described, even in the limit $r\to 0$, by a small number of spatial harmonics. However, we show that for $\zeta>\zeta_t$ the Fourier transform of $\mathbf{p}$, even in the modulated state, goes to zero quickly with increasing wave vector $\mathbf{Q}$ provided $d<4$. This is an important issue. First if the Fourier transform of $\mathbf{p}$ did not go to zero more quickly than Q^{-m} as Q tends to infinity then it would follow that F_{2m+2} were infinite for this state. In consequence the actual free energy for this state would be infinity, not the small value deduced from $\bar{F}$ and it would be necessary to find a new minimum taking the effect of (at least) F_6 into account. However, as we show below the $\mathbf{p}(\mathbf{x})$ which minimizes $\bar{F}$ is small and infinitely differentiable so that this breakdown of the Landau expansion does not occur. In addition since the Fourier transform falls rapidly with increasing wave vector the modulated phase may be well described by a small number of spatial harmonics so that expanding it in a finite series of spatial harmonics is a reasonable procedure, provided enough terms are taken into account.

In particular $f_u\geq f\geq f-\tilde{\alpha}\tilde{f}_4$ where $\tilde{\alpha}>0$ and $\tilde{f}_4=\tilde{F}_4/V$ and $\tilde{F}_4$ is given by Eq. (2.6) evaluated for $\tilde{\mathbf{p}}=\tilde{\beta}\mathbf{p}$, $\tilde{w}=w$, $\tilde{\Delta}=\Delta$, and $\tilde{\zeta}=\zeta_t$. Choosing $\tilde{\alpha}\tilde{\beta}^3=1$, $\tilde{\alpha}\tilde{\beta}^4=\zeta/\zeta_t$ and substituting in Eq. (2.4) we find

$$f_u-\tfrac{1}{2}r\langle p^2\rangle\geq(\zeta_t/\zeta)\tfrac{1}{2}[(1-\Delta)\langle\,|\nabla\cdot\mathbf{p}\,|^2\rangle +(1+\Delta)\langle\,|\nabla\times\mathbf{p}\,|^2\rangle +\langle\,|\nabla_N\mathbf{p}\,|^2\rangle] . \quad (2.19)$$

As $\langle p^2\rangle$ has already been shown to be bounded all (first) derivatives of $\mathbf{p}$ are square integrable and $\langle\,|\nabla\mathbf{p}\,|^2\rangle$ goes to zero as r goes to zero.

If $d<4$ square integrability of (first) derivatives of p implies that if there is a singularity in $\nabla\mathbf{p}$ then $|\,\mathbf{p}\,|^2$ diverges less quickly than $\nabla\mathbf{p}$ at that singularity as $\nabla\mathbf{p}$ must tend to infinity more slowly than $\delta X^{-d/2}$ where δX is the distance from the singularity. Therefore the terms in $(\nabla\mathbf{p})^2$ dominate the contribution to the free energy near the singularity. As all the terms in $\nabla\mathbf{p}$ in the free energy are positive it follows that if $\nabla\mathbf{p}$ has a singularity, the free energy can be decreased by smoothing that singularity, say by letting

$$\mathbf{p}(\mathbf{X})=\int d\mathbf{X}'\,p(\mathbf{X}')(2\pi\sigma)^{-d}\exp(-\,|\,\mathbf{X}-\mathbf{X}'\,|^2\sigma^{-2}) , \quad (2.20)$$

with σ small. This is because if σ is sufficiently small the most important effect of this convolution will be to make the derivatives of p finite, decreasing the contribution to the free energy. It follows therefore that the $\mathbf{p}$ which minimizes $\bar{F}$ and its first derivatives must be finite everywhere.

It is then easy to see provided $\mathbf{p}$ and its first derivative are finite (again from the minimization condition) that p satisfies the Euler equation

$$D_{\alpha\beta}p_\beta=H_\alpha(\{p_\beta,\partial_\beta p_\gamma\}) . \quad (2.21)$$

Here and below sums are implied over repeated indices and

$$D_{\alpha\beta}=\tfrac{1}{2}[(1+\Delta)(\delta_{\alpha\beta}\nabla^2-\partial_\alpha\partial_\beta)+(1-\Delta)\partial_\alpha\partial_\beta+\delta_{\alpha\beta}\nabla_N^2] , \quad (2.22)$$

$$H_\alpha=4up^2p_\alpha+2wp_\alpha\nabla\cdot\mathbf{p}-2wp_\beta\partial_\alpha p_\beta , \quad (2.23)$$

and $\delta_{\alpha\beta}$ is the Kronecker δ function, unity for $\alpha=\beta$ and zero otherwise. The formula for H_α was obtained by a variational calculation on the FEF, Eqs. (2.1)–(2.3). Note that right-hand side is everywhere finite as it contains only $\mathbf{p}$ and its first derivatives. This is adequate to demonstrate that $\mathbf{p}$ is infinitely differentiable. In particular, consider any small hypercubical region, $\bar{V}$, defined by $|\,X_\alpha-\tilde{X}_\alpha\,|<L$ for all α. The function p must be finite and differentiable on the boundary of this region and must satisfy Eq. (2.19) inside this region. Suppose $\mathbf{p}$ is specified on the surface of this region; we may rewrite (2.20) as

$$p_\alpha(\mathbf{X})=\int d\mathbf{X}'\,\bar{G}_{\alpha\beta}(\mathbf{X},\mathbf{X}')H_\beta(\{p'_\beta(\mathbf{X}'),\partial_\beta p'_\gamma(\mathbf{X}')\}) +\mathbf{p}^0(\mathbf{X}) , \quad (2.24)$$

where $\mathbf{p}=\mathbf{p}'$ and $\mathbf{p}^0$ is given by

$$p^0_\alpha(\mathbf{X})=\oint_S p_\beta(\mathbf{X}')\frac{\partial\bar{G}}{\partial n}d\mathbf{S}' .$$

Here $\partial/\partial n$ is the normal derivative at the surface S (directed outwards from inside the volume $\bar{V}$) and $\bar{G}$ is the Green's function for D, given that $\bar{G}(\mathbf{X},\mathbf{X}')=0$ for $\mathbf{X}$ on the boundary of the system. It is easy to verify by explicit construction that (a) $\mathbf{p}^0$ is infinitely differentiable in the interior of the hypercube, (b) all integrals of the absolute value of $\bar{G}$ and its first derivatives are finite and tend to zero as the size of the hypercube (L) tends to zero, and (c) any integral of the form $\int d\mathbf{X}'\,\bar{G}(\mathbf{X},\mathbf{X}')h(\mathbf{X}')$ where h is infinitely differentiable is also infinitely differentiable inside $\bar{V}$. Now consider the sequence $\mathbf{p}^{(m)}$, $m=0,\ldots,\infty$, where $\mathbf{p}^{(m)}$ is the right-hand side of (2.24) with $\mathbf{p}'=\mathbf{p}^{(m-1)}$ on the left-hand side. It follows from (a) and (c) that the terms in this sequence are infinitely differentiable inside $\bar{V}$, and from (b) and the fact that $\mathbf{p}$ and its derivatives are bounded on the surface that for small enough L this sequence is absolutely and uniformly convergent inside $\bar{V}$. Therefore $\mathbf{p}$ must be infinitely differentiable inside any sufficiently small hypercube. As this hypercube is arbitrary $\mathbf{p}$ must be infinitely differentiable everywhere. It follows that $\mathbf{p}(\mathbf{Q})$ tends to zero more quickly than any power of the wave vector Q, for $Q \gg r^{1/2}$.

Therefore for $\zeta_t < \zeta < 0$ the lowest free-energy state of the system is modulated but has a Fourier transform with most of the weight of $\int d\mathbf{Q}\,|\,\mathbf{p}(\mathbf{Q})\,|^2$ coming from Q less than or of the order of $|\,r\,|^{1/2}$. Unless ζ is small there is no reason to suppose that the fundamental wave vector is on a scale much less than $r^{1/2}$, as a range of wave vectors with $Qr^{-1/2}$ finite are unstable. We expect in consequence that the modulated state will be well described by a small number of modes in this region. This is confirmed by the fact that Blankschtein *et al.*[8] have found a two-harmonic modulated state with energy less than the uniform state for $\zeta=-0.048$, very close to the actual transition value $\zeta=0$. In any case as p is small and slowly varying the Landau expansion (i.e., neglecting $F_m, m>4$) is legitimate, at least sufficiently close to the transition ($r=0$) for $\zeta>\zeta_t$.

These bounds, of course, cease to apply when $\zeta \to \zeta_t$. However as $\zeta\to\zeta_t$ the free energy considered above is inadequate, more terms must be considered in the Landau expansion. This is done by adding F_6. If F_6 is not bounded below there will be a first-order transition to some other state for $\zeta>\zeta_t$. Assuming therefore that F_6 is bounded below, we also expect that the Fourier transform of p will tend to zero very rapidly as Q tends to infinity in this case, in extension of the discussion above.

C. Behavior near the uniform-modulated phase transition

We now consider the behavior of the system when ζ is close to $\zeta_u=0$. In particular we examine the behavior of f as $\zeta\to 0$ from below, i.e., as the transition is approached (ζ will be varied by varying u, keeping r, Δ, and w constant). We see immediately from Eq. (2.3) that

$$\partial f/\partial\zeta = w^2[2(1-\Delta)]^{-1}\langle\,|\,\mathbf{p}\,|^4\rangle\ .$$

Thus if the transition is to be first order in the sense that $\partial f/\partial \zeta$ is discontinuous across the transition it follows that as ζ goes to zero from below the lowest free-energy state must have $\langle\,|\,\mathbf{p}\,|^4\rangle \neq M^4$ or $\langle(\,|\,\mathbf{p}\,|^2-M^2)^2\rangle\neq 0$. However, it is easy to see that $\langle(\,|\,\mathbf{p}\,|^2-M^2)^2\rangle$ is bounded so that this state must have

$$\begin{aligned} f'V &= fV - V(\zeta w^2[2(1-\Delta)]^{-1}\langle(\,|\,\mathbf{p}\,|^2-M^2)^2\rangle + f_u) \\ &= V_N\int d\mathbf{x}\,\tfrac{1}{2}\left[(1-\Delta)\left[\nabla\cdot\mathbf{p}+\frac{w}{(1-\Delta)}(\,|\,\mathbf{p}\,|^2-M^2)\right]^2 + (1+\Delta)\,|\,\nabla\times\mathbf{p}\,|^2 + |\,\nabla_N\mathbf{p}\,|^2\right] \end{aligned} \qquad (2.25)$$

tending to zero as $\zeta\to 0$. As all these terms are nonnegative this is a very stringent condition. We have not been able to find any function $\mathbf{p}$ which satisfies (2.25) with $\langle(\,|\,\mathbf{p}\,|^2-M^2)^2\rangle\neq 0$ and speculate that no such $\mathbf{p}$ exists.

It is, however, still possible to put bounds on the behavior of f as $\zeta\to 0$. This is done (as above) by assuming $\nabla\times\mathbf{p}=0$ and writing[16] $\mathbf{p}=(1-\Delta)w^{-1}\nabla\ln(\psi)$ where ψ is assumed to depend only on $\mathbf{x}$ and not $\mathbf{x}_N$. Restricting $\mathbf{p}$ to have this form leads to the simplification

$$f'V = \frac{1}{2}\frac{(1-\Delta)^3}{w^2}V_N\int d\mathbf{x}\,\Gamma^2(\psi) \qquad (2.26)$$

where $\Gamma(\psi)=(\kappa^2-\psi^{-1}\nabla^2\psi)$ and $\kappa=|\,r\,|^{1/2}[2(1-\Delta)]^{-1/2}$. For f' to be zero requires $\nabla^2\psi=\kappa^2\psi$ everywhere except when $\psi\to\infty$. However, it is easy to see (as above) that for $n<4$ a region in which $\psi\to\infty$ has infinite free energy so that $\nabla^2\psi=\kappa^2\psi$ everywhere. Similarly we see that ψ can not be zero. It is now easy to construct states which have $f'=0$ and $|\,\mathbf{p}\,|^2\neq M^2$. Consider

$$\Psi(\mathbf{x}) = \int d\hat{\mathbf{\Omega}}'\,\Psi(\hat{\mathbf{\Omega}}')\exp(\kappa\mathbf{x}\cdot\hat{\mathbf{\Omega}}') \qquad (2.27)$$

where $\hat{\mathbf{\Omega}}'$ is a n-dimensional unit vector and the integral is with the usual weighting for solid angles. Then provided Ψ is non-negative and noninfinite it is clear that the conditions above are satisfied for finite $\mathbf{x}$. However, it is also clear from a steepest descent analysis of (2.27) that for large enough x, $\nabla\ln(\psi)$ tends quickly to $\kappa\hat{\mathbf{x}}$ in almost all directions $\hat{\mathbf{x}}$ so that $\langle(\,|\,\mathbf{p}\,|^2-M^2)^2\rangle=0$. We have not been able to construct potentials ψ which satisfy the conditions above and have $\langle(\,|\,\mathbf{p}\,|^2-M^2)^2\rangle\neq 0$.

The free energy for $\zeta<0$ can be bounded by any trial potential ψ. In order to obtain a good bound when $\zeta\to 0$ we have considered a potential in which the contributions to f' occur only at a small number of points and the contributions to $\zeta\langle(\,|\,\mathbf{p}\,|^2-M^2)^2\rangle$ occur along surfaces between the points. Thus as the separation between the points grows the importance of the favorable terms grows relative to the importance of the unfavorable term. In particular consider the potential

$$\psi = \sum_i \bar{K}_{(n-2)/2}(\kappa\,|\,\mathbf{x}-\mathbf{x}_i\,|\,) \qquad (2.28)$$

where the $\mathbf{x}_i$ form an infinite lattice and $\bar{K}(\tilde{x})$ is the potential (ψ) which minimizes the free energy of Eq. (2.26) above subject to the conditions that (a) $\bar{K}$ is rotationally invariant, (b) $\bar{K}(\,|\,\tilde{x}\,|\,)$ tends to zero as $\tilde{x}$ goes to infinity, and (c) $\nabla\bar{K}=0$, $\bar{K}\neq 0$ when $\tilde{x}=0$. There is an undetermined constant in $\bar{K}$. As shown below, for large $\tilde{x}$, $\bar{K}(\tilde{x})$ tends rapidly to a constant times $K_{(n-2)/2}(\mathbf{x})$, the associated Bessel function of the second kind of order $(n-2)/2$. The undetermined constant in $\bar{K}$ will be chosen so that this constant is unity. Close to the lattice points (within distances of order κ^{-1}) there are contributions to f'; however, these contributions fall off rapidly with increasing distance. Away from the lattice points the major contributions to the free energy come from $\zeta\langle(\mathbf{p}^2-M^2)\rangle$.

To demonstrate these facts we note, from Eq. (2.26), using the variational principle, that

$$d\Gamma/dx = 2w(1-\Delta)^{-1}\mathbf{p}\cdot\hat{\mathbf{x}}\Gamma$$

with $\mathbf{p}=(1-\Delta)w^{-1}\psi^{-1}\nabla\psi$. However, $\psi=\bar{K}$ is, by assumption, a decreasing function of $|x|$ so that Γ decreases rapidly with increasing x. Therefore, the contributions to f' also decrease rapidly with increasing x. If Γ is small the equation for ψ approaches Bessel's equation so $\bar{K}$ must approach the Bessel function. Therefore the asymptotic expansion of the Bessel function can be used to determine $\mathbf{p}$. For large x the Bessel function[17] $K(x)\sim x^{-1/2}e^{-x}$ tends to zero exponentially. It follows that for large x $\mathbf{p}=-(1-\Delta)w^{-1}\kappa(1+1/2x+\cdots)\hat{\mathbf{x}}$, which points in for $w>0$. Note that for large x the magnitude of the order parameter is nearly the constant M. However, it is clear that the p^2 implied by this potential does not equal M^2 within a distance of order κ^{-1} of the boundaries of the Wigner-Seitz cell of the lattice, i.e., near points which are equidistant from two or more nearest lattice points. Therefore if the lattice points are much more than κ^{-1} apart the free energy of this texture, shown for $2-d$ triangular lattice in Fig. 2, can be calculated approximately.

With the scaling transformation $\mathbf{x}\to\kappa^{-1}\mathbf{x}$, the free energy f', Eq. (2.26), becomes

$$f'V=\frac{(1-\Delta)^3}{2w^2}V_N\kappa^{4-n}F_c ,$$

where (2.29)

$$F_c=\int d\mathbf{x}(1-\psi^{-1}\nabla^2\psi)^2 .$$

Therefore for $\zeta\to 0$ and large $|\mathbf{x}_i-\mathbf{x}_{i'}|$ we find the difference in the free energy from the uniform free energy for this texture is approximately

$$F/V\sim v^{-1}|f_u|(F_c\kappa^{-n}-|\zeta|R^{n-1}F_w^L\kappa^{-1}) , \quad (2.30)$$

where v is the (average) volume per lattice site and R is the distance between the lattice points. The difference in the free energy within the core from the uniform free energy (i.e., the value of $f'-f_u$ when $\psi=\bar{K}$) is given by $F_c f_u\kappa^{-n}$ and the difference in the free energy of the wall from the uniform free energy (the edge of the Wigner-Seitz cell) is $|\zeta|R^{n-1}F_w^L f_u\kappa^{-1}$ given by $\zeta\langle(\mathbf{p}^2-\mathbf{M}^2)^2\rangle$. The free energy of the wall, proportional to $|\zeta|$, depends on the lattice and will be discussed further below. This approximation becomes exact when the lattice spacing is much larger than κ^{-1} and ζ is small. If we now consider the scaling transformation $\mathbf{x}_i\to(\lambda\kappa)^{-1}\mathbf{x}_i$ we find

$$F/V\sim v^{-1}\lambda^{-n}|f|_u[F_c-|\zeta|F_w^L(R\lambda\kappa)^{(n-1)}] , \quad (2.31)$$

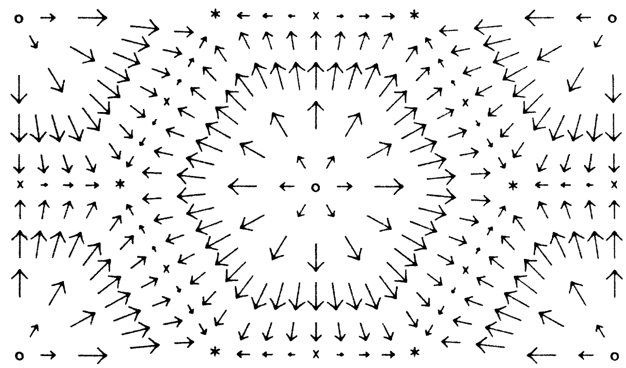

FIG. 2. Two unit cells of the triangular lattice for proposed modulated phase showing the Wigner-Seitz cell. In two dimensions there are vortices at the lattice site (○) at the center, at the corners (✱), and at the center of the sides (×). A representation of the magnitude of the order parameter is shown. The wall of width κ^{-1} is formed along the sides.

which, when minimized with respect to λ, yields

$$\lambda=\kappa^{-1}R^{-1}[|\zeta|F_w^L/(nF_c)]^{-1/(n-1)} , \quad (2.32)$$

so that $\lambda\to\infty$ as $\zeta\to 0$. The free energy is given by

$$F/V\sim v^{-1}R^n|f_u|(1-n)[|\zeta|F_w^L/(nF_c)]^{n/(n-1)} . \quad (2.33)$$

We now calculate F_w^L and F_c. It is easy to see, for example from the asymptotic expansion of the Bessel function, that in a region nearly equidistant from two lattice points the order parameter is given by

$$\mathbf{p}(\mathbf{x})=-\mathrm{sgn}(w)M[\hat{\mathbf{x}}'\tanh(x'\kappa\cos\theta)\cos\theta+\hat{\mathbf{y}}'\sin\theta] .$$

Here $\hat{\mathbf{x}}'$ is a unit vector normal to the equidistant surface, x' is the distance from this surface, and $\hat{\mathbf{y}}'$ is a unit vector in the plane of this surface pointing away from the lattice points. The angle θ is the angle between $\hat{\mathbf{x}}'$ and the line from the lattice point to the part of the wall under consideration. The direction of the order parameter changes by an angle $\pi-2\theta$ going through the wall. Substituting the order parameter $\mathbf{p}$ given above into $\zeta\langle(|\mathbf{p}|^2-M^2)^2\rangle$ yields

$$\zeta\langle(|\mathbf{p}|^2-M^2)^2\rangle\sim|\zeta|v^{-1}\kappa^{-1}F_w^LR^{n-1} , \quad (2.34)$$

$$R^{n-1}F_w^L=\int d\Omega\left|\frac{dA}{d\Omega}\right|f_w(\theta) , \quad (2.35)$$

where the integral is over all solid angles Ω, $dA/d\Omega$ is the area of the boundary of the Wigner-Seitz cell per unit solid angle, and $f_{w(}\theta)$ is the dimensionless free energy of the wall per unit area, given by

$$f_w(\theta)=\cos^3\theta\int_0^\infty d\tilde{x}\cosh^{-4}(\tilde{x})=\tfrac{2}{3}\cos^3\theta , \quad (2.36)$$

where $\tilde{x}=\kappa x'\cos\theta$. Clearly the integral over solid angles depends on the nature of the lattice. For one side of the wall of the triangular lattice $F_w^L=0.1458$. Thus the free energy of the entire wall is $0.83\zeta R|f_u|\kappa^{-1}$.

It is clear from these formulae that the lattice which minimizes this (negative) free energy is that which maximizes $\omega = v^{-1}R^nF_w^L$. Clearly ω is less than its value for a sphere $\omega_s(n) = \frac{4}{3}nS_n^{-1/(n-1)}$. We believe that the maximum value for ω in two dimensions is the value for a simple triangular lattice and that the maximum value for ω in three dimensions is that for a close-packed lattice. As these values are lower bounds within 10% of the upper bound they can not be far off, even if they are not exact.

We have calculated the free energy within the core numerically for $n=2$, 3, as follows. As $\lambda \to \infty$, $\mathbf{p}$ in the vicinity of the lattice points $\mathbf{x}_i$ tends to a spherically symmetric solution. Assuming

$$\mathbf{p} = (1-\Delta)^{1/2} |r|^{1/2} w^{-1} \hat{\mathbf{x}} g(|x|)/|x|$$

and rescaling x by $(1-\Delta)^{1/2}|r|^{-1/2}$ and substituting into $\bar{F}$ Eq. (2.6), we find, by the variational principle

$$2(2-\bar{\epsilon})g + (6-2\bar{\epsilon})g^2 + 2(1+\zeta)g^3 - \bar{\epsilon}g' - g'' - e^{2z}g = 0 , \tag{2.37}$$

with the difference in the free energy within the core and the uniform free energy, with n components, given by $|f_u|\kappa^{-n}V_NF_c$ with

$$F_c = S_n \int dz\, e^{-\bar{\epsilon}z}[g'^2 + V(g) - e^{2z}g^2] . \tag{2.38}$$

These equations are identical to (2.14) and (2.15) except for the term proportional to e^{2z} ($z=\ln x$) which appears as a result of including the term proportional to r in the free energy. The zero for z has been chosen so the coefficient of e^{2z} is unity. We have solved this equation numerically for $\zeta=0$ [$w^2=2u(1-\Delta)$], subject to the constraint that $g \to 0$ as $|x| \to 0$ and $|x| \to \infty$ or $z \to \pm\infty$. This was done by assuming a solution of the form $g = A_0\exp(2z)$ as $z \to -\infty$, i.e., $\mathbf{p} \propto \mathbf{x}$ as $x \to 0$. By adjusting the value of A_0 the condition as $z \to +\infty$ can be satisfied. The values of F_c were found to be $F_c(n=2) \sim 7.4$ and $F_c(n=3) \sim 17.0$.

It should be noted that when Δ is close to -1 we expect that the details of the solution will be modified because it will be favorable near the lattice points to have nonzero $\nabla \times \mathbf{p}$, decreasing both the free-energy cost of the vortex cores and the lattice constant of the resultant lattice. It is even possible that the nature of the modulated phase will change when Δ is sufficiently close to -1.

This calculation, together with the bounds of $|\mathbf{p}|^2$ imply that the difference between the uniform free energy and the actual free energy for $\zeta<0$ is bounded from below as $\zeta \to 0$ by a power law ($|\zeta|^{n/(n-1)}$) and from above by another power law ($|\zeta|$). We note that any bound for $n \to n-1$ is also a bound. However it is obvious from these formulae and Eq. (2.35) above that the bound for $n-1$ is greatly inferior to that for n as $\zeta \to 0$. This disproves the possibility that the transition, like a nucleation transition,[9] has an exponential dependence on the control parameter, ζ.

We speculate that $\bar{F} = Vf_u - \text{const} \times |\zeta|^{n/(n-1)}$ is in fact the correct asymptotic power-law behavior for the minimum of the free energy and the state $\mathbf{p}$ which minimizes the $\bar{F}$ as $\zeta \to 0$. In particular for $n>2$ we have not been able to find any states for which the negative contributions to the free energy increase as a larger power of the lattice size nor for which the total positive contributions to the free energy per unit cell decreases without bound with increasing lattice constant. We remark that for $n=2$ a phase like the "striped" phase discussed by Langer and Sethna[13] with stripes of widths L would have a free energy per unit volume of the form $f_u - |\zeta| f_w L^{-1} + \frac{1}{2}J(\Delta)L^{-2}$. Minimizing with respect to L we find the difference between the minimum free energy and the uniform phase scales in the same way, ζ^2, for both the hexagonal state we have discussed and this striped phase. Thus to determine the nature of the modulated phase the simple scaling arguments which apply for $n>2$ cannot be used. Rather it would be necessary to calculate with some precision the constant multiplying the ζ^2 term in the free energy, minimizing it over the possible textures of the order parameter (as a function of Δ). We will not carry out this calculation. Given the similarity between the free energies of the two-harmonic approximations[8] to phases with the same symmetries for $\Delta=0$ and larger negative ζ we expect that the differences between the free energies of the two phases is not large and that approximate calculations are therefore hard to interpret, at least for $\Delta=0$.

In summary we envisage a behavior somewhat like that suggested in Ref. 9, a star burst of modes with the Fourier transform of $\mathbf{p}(\mathbf{Q})$, tending to zero only slowly for a range of $|\zeta|^{-1/(n-1)} < r^{1/2}Q^{-1} < 1$. However, we expect this behavior only for small ζ and only for $Qr^{1/2}$ small, as ζ becomes more negative the range of $|\mathbf{Q}|$ over which $\mathbf{p}(Q)$ decreases slowly will decrease, as will the number of harmonics necessary to give a good description of the actual physical state.

D. Range of validity for mean-field theory

In general it is expected that the mean-field approximation will be legitimate provided that the order parameter is small enough (so that higher-order terms in the Landau expansion are not important) and provided the nonlinear terms are small enough so that the effects of fluctuations are small, i.e., a "Ginzburg" criterion is satisfied; $u(1-\Delta^2)^{-2}$, $w^2(1-\Delta^2)^{-3} \lesssim |r|^{-\epsilon/2}\Lambda^{\epsilon}$ where Λ is the maximum wave vector for which the description given above is legitimate. In this case, however, the range of validity is smaller than this, for small ζ.

The free energy which we are studying is very extraordinary as a wide variety of defects cease to have positive free energy and begin to have negative free energy along the line $\zeta=0$. In particular any order-parameter texture which can be written as the logarithmic gradient of a function of the form of (2.27) has positive free energy for $\zeta>0$ and negative free energy for $\zeta<0$. Such textures includes, *inter alia,* wall defects in which the order parameter rotates through an arbitrary angle and vortices. It is easy to see that when F_6 is included in the free-energy expansion then (except for very special values of the parameters in F_6) it is no longer true that all such defects have zero free energy for the same value of ζ. Of course as $r \to 0^-$ the magnitude of the order parameter and its gradients tend to zero for all states which need to be considered near $\zeta=0$ and $n<4$. Thus the differences between the free energies of the various defects will be very small as $r \to 0^-$ and, therefore will be irrelevant in this limit for any nonzero, specified value of ζ. However, for any specified $r<0$ there will be a ζ so small that the contribution to the free energy of various defects coming from F_6 will dominate the contribution from ζ. Therefore there will always be some small region near the uniform-modulated phase transition in which the F_6 terms play an important role in determining the nature of the modulated phase (and even the order of this transition). Therefore in this region some of the parameters in F_6 are "dangerous" irrelevant variables, and the discussion above must be modified to account for them.

In addition for small ζ, and for F_6 sufficiently small so that it can be ignored, the states discussed above are unstable to thermal fluctuations. In particular, consider the case $n=d$. We have shown above that there are states with point defects at arbitrary positions in the volume. Each such state has a free energy of the form

$$V(f_u \kappa^{-d} F_c \rho_D + \zeta \kappa^{-1} \overline{A} \rho_D^{1/d}) ,$$

where ρ_D is the density of defects and $\overline{A}$ is a configuration-dependent factor of order one provided the defects are, at least, a distance κ^{-1} apart. Clearly, therefore if ζ is sufficiently negative then the lattice discussed above will be stable under thermal fluctuations. If $|\zeta|$ is sufficiently small (whether ζ is positive or negative) then fluctuations will be important and we expect a gas (or liquid) of defects. However, if ζ is sufficiently positive the long-range interactions between defects reflected in the $\zeta \overline{A} \rho_D^{1/d}$ term are again important so that there are no defects in equilibrium. To get a rough idea of the region in which these various terms are important we first ignore the defect interaction term. We then expect, from the usual treatment of statistical mechanics, that the density of defects will be

$$\rho_D^0 \sim \kappa^{-d} \exp(-\kappa^{-d} f_u F_c / T) .$$

When the interaction term becomes important at this density there will be changes in the behavior. Therefore for the mean-field theory to be legitimate we require

$$|\zeta| \rangle \tilde{A} \exp[-\kappa^{-d} f_u F_c (1-d^{-1})/T] ,$$

where $\tilde{A}$ is a constant of order 1.

III. RENORMALIZATION GROUP

In this section we will give a renormalization-group[1] (RG) calculation for the properties of this model, in an expansion in $\epsilon=4-d$ where d is the spatial dimension. This calculation consists of successively eliminating the spatially quickly varying part of the order parameter and then rescaling lengths and the order parameter so that the space on which the system is defined is essentially unchanged.

The free energy $\overline{F}$, Eq. (2.3), can be written[8] in Fourier space as $\overline{F}=F_0+F_1$ where

$$F_0 = \int_{\mathbf{Q}} (\{[r+(\Delta_1+\Delta)q^2+\Delta_3 q_N^2]\delta_{\alpha\beta} - 2\Delta q_\alpha q_\beta\} p_\alpha(\mathbf{Q}) p_\beta(\mathbf{Q})) , \qquad (3.1)$$

and

$$F_1 = iw \int_{\mathbf{Q}} \int_{\mathbf{Q}'} [q_\alpha p_\alpha(\mathbf{Q}) p_\beta(\mathbf{Q}') p_\beta(-\mathbf{Q}-\mathbf{Q}')] , + u \int_{\mathbf{Q}} \int_{\mathbf{Q}'} \int_{\mathbf{Q}''} [p_\alpha(\mathbf{Q}) p_\alpha(\mathbf{Q}') p_\beta(\mathbf{Q}'') \times p_\beta(\mathbf{Q}-\mathbf{Q}'-\mathbf{Q}'')] . \qquad (3.2)$$

Here $p(\mathbf{Q}) = \int d\mathbf{X}\, e^{i\mathbf{Q}\cdot\mathbf{X}} p(\mathbf{X})$, and $\Delta_1=\Delta_3=1$.

The wave vector $\mathbf{Q}$ is $\mathbf{Q}=(\mathbf{q},\mathbf{q}_N)$ where $\mathbf{q}$ is a vector in the n-component space spanned by $\mathbf{p}$ and $\mathbf{q}_N$ is a $(d-n)$-component vector in the orthogonal subspace and the integral

$$\int_{\mathbf{Q}} \equiv (2\pi)^{-d} \int_{|\mathbf{Q}|<\Lambda} d\mathbf{q}\, d\mathbf{q}_N .$$

Note that all fluctuations with $|\mathbf{Q}|>\Lambda$ have been eliminated from the free energy. Expectation values are defined in the usual way as functional integrals with the weight $\exp(-F)$. The RG calculation is performed by[1,7,8] eliminating fluctuations in an elliptical shell given by

$$(q/b)^2+(q_N/a)^2>\Lambda^2>q^2+q_N^2$$

with $a,b>1$, treating F_0 exactly and using a perturbation expansion in F_1. The wave vectors $\mathbf{q}$ and $\mathbf{q}_N$ are then rescaled anisotropically[7] by the transformation $\mathbf{q}'=\mathbf{q}b$ and $\mathbf{q}'_N=\mathbf{q}_N a$ with $b,a>1$ and the order parameter p is rescaled by $p(q',q'_N)=\phi p(qb,q_N a)$ where ϕ is the spin rescaling factor determined below. The propagator,

$$G_{\alpha\beta}(\mathbf{Q}) \equiv V^{-1} \langle p_\alpha(\mathbf{Q}) p(-\mathbf{Q})_\beta \rangle_0 ,$$

where $\langle\ \rangle_0$ indicates the expectation value with the unperturbed free energy F_0 is given by

$$G_{\alpha\beta}(Q) = \frac{T_{\alpha\beta}(q)}{r+(1+\Delta)q^2+\Delta_3 q_N^2} + \frac{L_{\alpha\beta}(q)}{r+(1-\Delta)q^2+\Delta_3 q_N^2} \qquad (3.3)$$

where $L_{\alpha\beta}(q)$ is the longitudinal projection operator, $L_{\alpha\beta}(q)=q_\alpha q_\beta/q^2$, and $T_{\alpha\beta}(q)$ is the transverse projection operator, $T_{\alpha\beta}(q)=\delta_{\alpha\beta}-L_{\alpha\beta}(q)$. The parameter Δ is assumed to be $O(1)$ and is restricted to $-1\le\Delta\le 1$ so that the free energy is stable. The parameters r, $y=w^2$, and u are assumed to be small.

A. Recursion relations

The recursion relations can be obtained from a diagrammatic expansion of $\overline{F}$. The contributions to the parameters r, y, and u are evaluated from the Feynman diagrams obtained doing a perturbation expansion in powers of F_1 around the unperturbed free energy F_0 and are evaluated using the propagator (3.3). The diagrams are constructed from the w- and u-type vertices given schematically in Fig. 3. Other contributions to the renormalized free energy of F are all of higher order in u, w, or ϵ. All contributions of lowest order in u, w, or ϵ have been included (see Fig. 4). Thus all the terms which have been neglected are clearly small compared to at least one of the given terms. There are numerous diagrams constructed from w- and u-type vertices and combinations of w and u vertices and evaluating them is an arduous task. Fortunately most of these calculations have been performed by Blankschtein *et al.*[8] and Aharony,[18] graphs involving u alone which contribute to the renormalization of u and Δ for $n=d=4-\epsilon$ by Aharony,[18] and graphs involving w as well as u by Blankschtein *et al.*[8] As we shall see below, these calculations are adequate for an understanding of the renormalization-group flows.

We have checked and employed their results. We will not comment in detail on their calculation except to remark that the evaluation of graphs involving w can be simplified, in comparison to the methods of Ref. 8. Similar tricks may decrease the labor in related problems. Consider a graph in which an external line is connected to a w-type vertex. For each w vertex in a fixed graphical topology there are three different such graphs as the gradient can be along any of the three lines attached to the w vertex. Consider the contribution to this graph in which the internal propagators are longitudinal, i.e., corresponding to the second term in Eq. (3.3). It is useful to sum immediately over the possible orientations of the w vertex (prior to summing over topologically equivalent graphs), yielding, for the contribution of the w vertex and the two longitudinal projection operators in the propagators,

$$iw[(q_\alpha q^2/4)-2q'_\alpha \mathbf{q}\cdot\mathbf{q}']q_\beta^+ q_\gamma^-(|q^+|\,|q^-|)^{-2} \qquad (3.4)$$

where $\mathbf{Q}$ is the wave vector of the external line and $\mathbf{Q}^\pm=(\pm\mathbf{Q}'-\mathbf{Q}/2)$ are the wave vectors along the internal lines. The subscript α is the vector index of the external lines and β and γ are the vector indices of the internal lines. The immediate consequence is that the contribution of the sum over all orientations of the w vertex for any graph in which two longitudinal propagators meet at a w vertex goes to zero as $\mathbf{q}$ goes to zero. If there are two or more w vertices attached to external lines at which two longitudinal propagators meet then simple extensions of the above argument show that the value of the sum of such graphs over all orientations of the w vertex goes to zero as the product of the q's along the attached external lines. We also note that graphs in which the gradient of the w vertex are along a line with a transverse propagator are trivially zero. This immediately eliminates from consideration a large number of graphs; for example the only graph which must be considered in the w^4 term in the recursion relation for u is that shown in Fig. 5. This compares to four (more complex) graphs required by the previous analysis.[8] It implies that none of the graphs calculated (except the u^2 contributions to Δ, the graphs of Fig. 5) need involve more than two transverse or two longitudinal propagators.

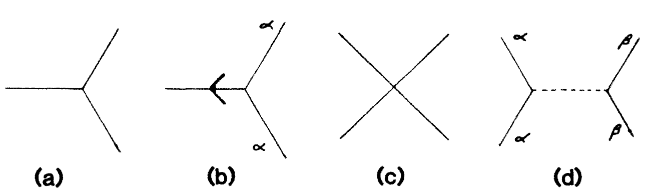

FIG. 3. (a) and (b) show two graphical representations of w-type vertices. The arrow in the leg of the (b) represents the leg along which we have $\nabla\cdot\mathbf{p}$. The u-type vertices are given in (c) and (d). The spin labeling is shown in (b) and (d).

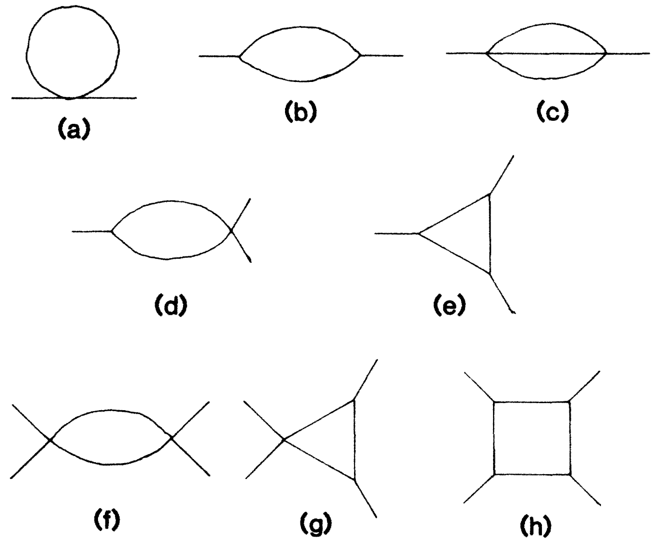

FIG. 4. The Feynman diagrams for the contributions to the recursion relations: (a) and (b) are contributions to r; (a), (b), and (c) contribute to Δ' and the spin and space rescaling factors. The graphs (d) and (e) contribute to w', and (g)–(h) to u'.

The ratio a/b was determined[8] by requiring that the renormalized coefficient of the term proportional to q_N^2, (Δ_3'), be unity. The order-parameter rescaling factor ϕ was determined by requiring that the renormalized coefficient of the q^2 term, (Δ_1'), be unity. The result is

$$\ln(a)=\{1+[X_1(\Delta)-X_3(\Delta)](y/2)+[Y_1(\Delta)-Y_2(\Delta)]u^2 + O(y^2,yu,u^3)\}\ln(b)\ . \qquad (3.5)$$

With this result along with the results given by Aharony[18] an order-parameter rescaling factor can be deduced. The result is

FIG. 5. Diagrams of (a) order w^2 contributing to r' and (b) w^4 contributing to u'. The wavy line indicates that this internal line contributes only the transverse part of the propagator and the solid internal line indicates only the longitudinal part of the propagator.

$$2\ln(\phi)=(d+2+X_1(\Delta)y+Y_1(\Delta)u^2+(4-n)\{[X_1(\Delta)-X_3(\Delta)](y/2)+[Y_1(\Delta)-Y_3(\Delta)]u^2\}+O(y^2,yu,u^3))\ln(b)\ , \tag{3.6}$$

where b is the momentum rescaling factor and the functions X_1, X_3, Y_1, and Y_3 are the results of graphical calculations which are given in Table I, insofar as they are required for discussion in this paper. Once this factor is determined the recursion relations in the parameter space (Δ,y,u) can be found to lowest order.

The renormalized parameter r', which has not been given in previous work, will now be obtained explicitly to $O(\epsilon)$. The graphs contributing to r' are proportional to w^2 [Figs. 6(a) and 6(b)] and u [Figs. 6(c) and 6(d)]. The graphs of order u are obtained by taking a u vertex and contracting two legs in all possible ways. The graphs of order w^2 are constructed by taking two w vertices and contracting pairs of legs in all ways that create connected graphs. From these diagrams (see Fig. 6) we find r' is the coefficient of $\delta_{\alpha\beta}$ in

$$\phi^2 b^{-n} a^{-d+n}\left[r+4u\delta_{\alpha\beta}\int_Q G_{\gamma\gamma}(\mathbf{Q})+8u\int_Q G_{\alpha\beta}(\mathbf{Q})+4w^2\int_Q G_{\alpha\beta}(\mathbf{Q})G_{\gamma\delta}(\mathbf{Q})q_\gamma q_\delta-4w^2\int_Q G_{\alpha\beta}(\mathbf{Q})G_{\gamma\delta}(\mathbf{Q})q_\gamma q_\beta\right]\ , \tag{3.7}$$

where sums over repeated indices are implied. The first term of (3.7) results from rescaling r. The integral proportional to u will be evaluated explicitly. Inserting $G_{\gamma\gamma}$ and summing over γ from 1 to n gives

$$\int_Q G_{\gamma\gamma}=\int_Q \frac{(n-1)}{r+(1+\Delta)q^2+\Delta_3 q_N^2}+\int_Q \frac{1}{r+(1-\Delta)q^2+\Delta_3 q_N^2}\ . \tag{3.8}$$

We will assume that the parameter $r\sim(T-T_c)$ is of order ϵ. The denominators in the above integrals are then expanded to first order in r. Evaluating these integrals[19] for $d=4$ dimensions we find

$$I_\pm \equiv \int \frac{q^{n-1}q_N^{3-n}dq\,dq_N}{(1\pm\Delta)q^2+\Delta_3 q_N^2}-r\int\frac{q^{n-1}q_N^{3-n}dq\,dq_N}{[(1\pm\Delta)q^2+\Delta_3 q_N^2]^2}$$
$$=(1-b^{-2})\frac{K_4[(1\pm\Delta)^{(2-n)/2}\Delta_3^{(n-2)/2}-1]}{(2-n)(1\pm\Delta)-\Delta_3}$$
$$-r(1\pm\Delta)^{-n/2}\Delta_3^{(n-4)/2}K_4\ln b\ , \tag{3.9}$$

where $K_4=S_4(2\pi)^{-4}$ and S_4 is the area of the 4-sphere, given in Sec. II B. Other contributions to r' can be evaluated similarly, yielding

$$r'=\phi^2 b^{-n}a^{-d+n}\left[r+\frac{4(n-1)}{n}\left[(n+2)u-\frac{y}{2\Delta}\right]I_+ +\frac{4}{n}\left[(n+2)u+\frac{y}{2\Delta}\right]I_-\right]\ . \tag{3.10}$$

To find the change in r with length scale in differential form, b is taken as e^l and $r'=r(l+\delta l)$. Then using Eq. (3.6) for ϕ in terms of b, and expanding the exponential in small displacements of l to $O(\delta l)$ and taking the limit as $\delta l\to 0$ with $n=d=4-\epsilon$, yields

$$\frac{dr}{dl}=(2+X_1 y+Y_1 u^2)r+2Y_4 u+Y_5 ru+2Y_6 y+Y_7 ry\ , \tag{3.11}$$

where the functions Y_4, Y_5, Y_6, and Y_7 are given in Table I.

Similarly the RG equations for (Δ,y,u) in differential form for arbitrary n are

$$\frac{d\Delta}{dl}=\Delta[(X_1-X_2)y+(Y_1-Y_2)u^2]+O(yu,y^2,u^3)\ , \tag{3.12}$$

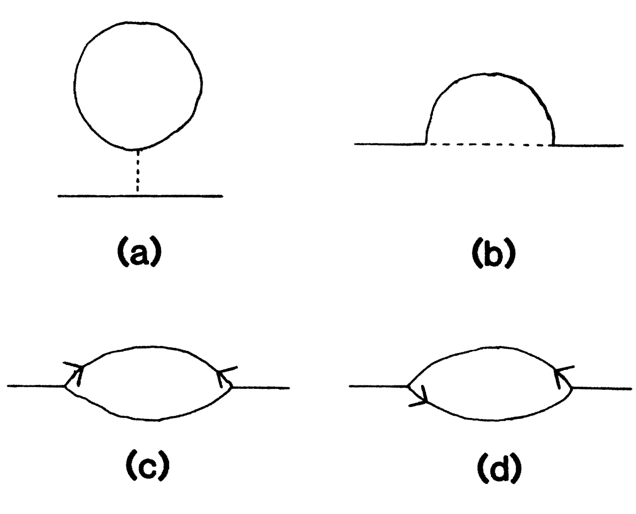

FIG. 6. The Feynman diagrams of order u^2 [(a) and (b)] and w^2 [(c) and (d)] which contribute to the renormalization of r.

TABLE I. The functions $X_i(\Delta)$ ($i=1-8$) and the functions $Y_i(\Delta)$ ($i=4-7$) for arbitrary n.

i	α_i	β_i	γ_i
1	$\frac{2}{n(n^2-4)\Delta^3}$	$[\frac{1}{2}(n^4-n^3)-n^2+5n-2]\Delta^3+2n\Delta^2$ $-[n^2+3n-2]\Delta-2n$	$[2n^3-5n+2]\Delta^3-3n^2\Delta^2$ $-[n^2-3n+2]\Delta+2n$
2	$\frac{2}{n(n^2-4)\Delta^4}$	$[\frac{1}{2}(-n^4+n^3)-4n+6]\Delta^3$ $-[2n^2+2n-6]\Delta^2-2\Delta-2$	$[2n^3-5+2]\Delta^3-3n^2\Delta^2$ $+(3n^2-6)\Delta^2-(2n-2)\Delta+2$
3	$\frac{2(n-1)}{n(4-n)(n-2)\Delta^3}$	$(n-2)\Delta^2+n\Delta+2$	$-(n-2)\Delta^2+n\Delta-2$
4	$\frac{8}{n(n-2)\Delta^2}$	$\frac{1}{2}[n^3-n^2-4n+6]\Delta^2-1$	$[n^2-3]\Delta^2-n\Delta+1$
5	$\frac{2}{n(n-2)\Delta^2}$	$[-n^2+4n-5]\Delta+n-2$	$[2n^2-7n+5]\Delta+3-n$
6	$\frac{4(n-1)}{n(n^2-4)\Delta^2}$	$[-3n^2+8]\Delta-2n$	$[n^2-8]\Delta+2n$
7	$\frac{(n^2-1)}{n(n^2-4)\Delta^3}$	$n\Delta+2$	$n\Delta-2$
8	$\frac{4}{n(n^2-4)\Delta}$	$[n^4+7n^3-16n^2-24n+32]\Delta-8n+8$	$[n^3+4n^2-32]\Delta+8n-8$

where $X_i=\alpha_i(\beta_i I_+ +\gamma_i I_-)$ and $I_\pm=(1\pm\Delta)^{-n/2}\Delta_3{}^{-(4-n)/2}$

$$Y_4=\frac{4(n-1)(n+2)}{n}J_+ +\frac{4(n+2)}{n}J_-$$

$$Y_5=\frac{4(n-1)(n+2)}{n}I_+ +\frac{4(n+2)}{n}I_-$$

$$Y_6=\frac{2}{n\Delta}J_- -\frac{4(n-1)}{n}J_+$$

$$Y_7=\frac{2}{n\Delta}I_- -\frac{4(n-1)}{n}I_+$$

where $J_\pm=K_4\left[\frac{(1\pm\Delta)^{(2-n)/2}\Delta_3^{(n-2)/2}}{(2-n)(1\pm\Delta)-\Delta_3}\right]$, $I_\pm=K_4(1\pm\Delta)^{-n/2}\Delta_3^{-(4-n)/2}$, $K_4=\frac{1}{8\pi^2}$

$$\frac{dy}{dl}=(\epsilon-2X_4u)y+[3X_1+2X_5+\tfrac{1}{2}(n-4)(X_1-X_3)]y^2+O(y^2u,yu^2)\ , \tag{3.13}$$

$$\frac{du}{dl}=\epsilon u-X_8u^2+[2X_1+X_6+\tfrac{1}{2}(n-4)(X_1-X_3)]yu-X_7y^2+O(u^3,yu^2,y^2u,y^3)\ . \tag{3.14}$$

Note that the X_i ($i=1,8$) are polynomials in n, $Y_i(i=1,2)$ are given only for $n=4$ and both are functions of Δ. It has not been necessary to calculate Y_3 as it does not appear in Eqs. (3.11)–(3.14). All X_i are positive for $-1<\Delta<1$ except X_2; ΔX_2 is negative for $-1<\Delta<1$. For the case $n=d$, X_3 does not appear in the above differential equations since it is associated with the $(n-d)$-dimensional subspace perpendicular to **p** and hence must not enter. The higher-order terms indicated in the differential equations for Δ, y, and u above will be neglected henceforth, except the yu^2 term of the y equation, which will be needed for reasons discussed below. When these terms are neglected the resultant nonlinear ordinary differential equations can be analyzed.

B. Fixed points

The fixed points are those values of the parameters (Δ,y,u) which are invariant under the RG transformation. These points (Δ^*,y^*,u^*) are found from Eqs. (3.12), (3.13), and (3.14) by setting the right-hand sides (rhs's) equal to zero. When $\Delta\to\pm1$, there are divergences in all the functions X_i and as $\Delta\to1$ there are divergences in Y_1 and Y_2. This case requires a somewhat different treatment which will be given separately below. There are three possible conditions for fixed points for $\Delta\neq\pm1$: (i) $y=u=0$, (ii) $y=0$ but $u\neq0$, and (iii) $y\neq0$ and $u\neq0$. First if $y=u=0$ then the rhs's of Eqs. (3.12)–(3.14) are zero for any Δ. This results in the trivial (Gaussian) fixed line. If $y=0$ but $u\neq0$ then (3.12) implies that Δ must be zero since (Y_1-Y_2) is never zero. Hence the fixed-point value for u is determined from (3.14). It has the usual Wilson-Fisher value

$$u^*=\epsilon/X_8(0)=\epsilon/[4K_4(n+8)]\ .$$

Finally if y is nonzero then (3.12) implies

$$y=\frac{-(Y_1-Y_2)u^2}{(X_1-X_2)}\ . \tag{3.15}$$

Turning our attention to Eq. (3.12) the following possibilities are considered: (i) $(Y_1-Y_2) \ll (X_1-X_2)$ which implies that $y \ll u^2$; (ii) $(Y_1-Y_2) \sim (X_1-X_2)$, which implies that $y \sim u^2$; and (iii) $(Y_1-Y_2) \gg (X_1-X_2)$ which would imply that $y \gg u^2$. The values of X_i and Y_i were calculated numerically for all Δ with $-1<\Delta<1$. It was found that (X_1-X_2) is always at least 1 order of magnitude larger than (Y_1-Y_2). Therefore condition (iii) never applies because (X_1-X_2) is greater than (Y_1-Y_2) for all Δ, so $y<u^2$ to lowest order in ϵ for any Δ. Since y is at most $O(u^2)$ the terms of order yu and y^2 in (3.14) are negligible near the fixed point. Thus the fixed-point value of u is $u^*=\epsilon/X_8(\Delta)+O(\epsilon^2)$. Since y^* is $O(u^2)$, y is at most $O(\epsilon^2)$.

The fixed-point values for Δ and y can now be determined. For $y\neq 0$, $y=O(\epsilon^2)$, the rhs of Eq. (3.13) can be zero only if $(\epsilon-2X_4u^*)$ is of order ϵ^2. Replacing u with $u^*=\epsilon/X_8(\Delta)$ shows that $(1-2X_4/X_8)=0+O(\epsilon)$. This determines Δ^* to order ϵ. It is found, for $n=d=4$, that $(1-2X_4/X_8)$ vanishes when $\Delta=0$ and when $\Delta=-\frac{2}{3}$. The quantity $(1-2X_4/X_8)$ reaches its maximum value of about 0.1 between $\Delta=0$ and $\Delta=-\frac{2}{3}$ (see Fig. 7). We note, however, that $\epsilon(1-2X_4/X_8)$ is very small (~ 0.1) throughout the region in which it is positive, and the slopes near the zeros are also small. In consequence it may be that the value of Δ^* (and even the existence of a Δ^*) will depend strongly upon the next-order terms, which are expected to be roughly $\epsilon^2/(n+8)\sim 0.1$ for $\epsilon=1$. We have not pursued a higher-order calculation. For $n=3$ and $n\simeq 2$ $(1-2X_4/X_8)=0$ only at one point for $\Delta^*(n=3)\simeq 0.22$ and $\Delta^*(n=2.05)\simeq 0.53$.

The y recursion relation determines the fixed-point values for Δ, and the recursion relation for Δ, Eq. (3.12), must be utilized to find y^*. From Eq. (3.15) it is found that if $\Delta<0$, y is less than zero because both (Y_1-Y_2) and (X_1-X_2) are less than zero. On the other hand if $\Delta^*>0$ $(Y_1-Y_2)<0$ but $(X_1-X_2)>0$ so $y^*>0$. The fixed points occurring in the $y=w^2>0$ region will be referred to as ferroelectric while those fixed points occurring in the $y<0$ will be referred to as polymeric. Now for $n=4$ substituting $\Delta^*=-\frac{2}{3}$, and $u^*=\epsilon/X_8(-\frac{2}{3})$ into (3.15) determines y^*. The results are $\Delta^*=-\frac{2}{3}$, $y^*=-5.443\times 10^{-4}\epsilon^2$ and $u^*=0.2492\epsilon$. We expect that this fixed point will be qualitatively the same for other n, provided it exists.

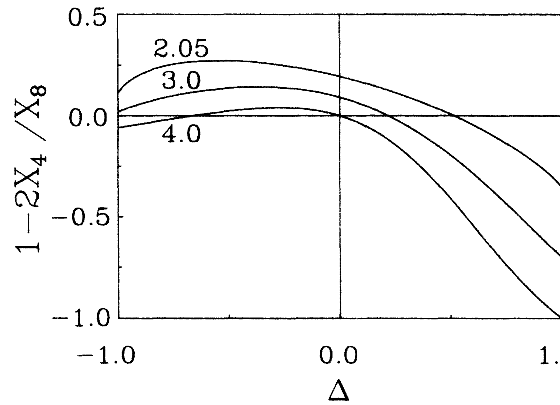

FIG. 7. Plot of $1-[2X_4(\Delta)/X_8(\Delta)]$ for $-1\leq\Delta\leq 1$ for $n=2.05$, 3.0, 4.0.

For $n=4$ there is also a $y^*\neq 0$ fixed point for $\Delta=O(\epsilon)$. As the nature of the fixed point changes when $\Delta=0$ it is interesting to determine the nature of the fixed point in the vicinity of $n=d=4$. To do this we will assume that $d=4-\epsilon$ and $n=4-g\epsilon$. This not only allows us to discuss this fixed point when it is near $\Delta=0$, which occurs for an interesting case, $n=d$, but also implies that knowledge of Y_1 and Y_2 for $n=d$ (which is available from the literature) suffices to determine the behavior. To determine the fixed point near $\Delta=0$, for $n=d=4-g\epsilon$ to lowest nontrivial order requires calculating the behavior of the X_i as $\Delta\to 0$. It is found that

TABLE II. The functions $X_i(\Delta)(i=1-8)$, $Y_1(\Delta)$, and $Y_2(\Delta)$ for $n=4$.

(1)	$X_1=\frac{1}{3}K_4(8-2\Delta+26\Delta^2)\frac{1}{(1-\Delta^2)^2}$
(2)	$\Delta X_2=\frac{1}{3}K_4(-7+4\Delta-25\Delta^2)\frac{1}{(1-\Delta^2)^2}$
(3)	$X_4=K_4(24-16\Delta+32\Delta^2)\frac{1}{(1-\Delta^2)^2}$
(4)	$X_5=K_4(7+\Delta)\frac{1}{(1-\Delta^2)^2}$
(5)	$X_6=K_4(24-8\Delta)\frac{1}{(1-\Delta^2)^2}$
(6)	$X_7=K_4(\frac{5}{2})\frac{1}{(1-\Delta^2)^2}$
(7)	$X_8=K_4(48-48\Delta+40\Delta^2)\frac{1}{(1-\Delta^2)^2}$
(8)	$Y_1=-32K_4^2(1+\Delta)\left[\frac{3}{2}+\frac{8}{3}\left[\frac{\Delta}{1-\Delta}\right]+\frac{19}{6}\left[\frac{\Delta}{1-\Delta}\right]^2+\left[\frac{\Delta}{1-\Delta}\right]^3\right]$
(9)	$Y_2=-32K_4^2(1+\Delta)^2\left[\frac{5}{6}\left[\frac{1}{1-\Delta}\right]+\frac{1}{3}\Delta\left[\frac{1}{1-\Delta}\right]^2+\frac{1}{2}\Delta^2\left[\frac{1}{1-\Delta}\right]^3\right]$

all X_i except X_2 are continuous in this limit; X_2 tends to $(7/3\Delta)K_4$. However, Eq. (3.12) still remains finite as ΔX_2 is finite. Actually it is a pleasant task to determine the limiting values for all X_i since they reduce to a such simple form for the case $n=4$ (see Table II). The term (Y_1-Y_2) is also finite and goes to $(-\frac{64}{3})K_4^2$ at $\Delta=0$. Equation (3.15) and the above limiting values determine $y^*=(\frac{64}{7})\Delta^* u^{*2}$. Since both u^* and Δ^* are $O(\epsilon)$, y^* is $O(\Delta\epsilon^2)$.

The value of Δ^* is determined principally by $\epsilon(1-2X_4/X_8)$ in the y recursion relation. It is easily shown that $X_8(\Delta=0)=2X_4(\Delta=0)$ for $n=4$ so that at $\Delta=0$ the term proportional to y in (3.13) vanishes. Therefore it is necessary to expand X_4/X_8 near $\Delta=0$ with $n=4-g\epsilon$ and to keep all terms which are of order ϵ or Δ. This yields

$$\frac{X_4}{X_8}=\tfrac{1}{2}+\tfrac{1}{6}\Delta-\tfrac{1}{24}g\epsilon \ . \tag{3.16}$$

The X_9 term is the $O(yu^2)$ of (3.13) and cannot be neglected for the $\Delta=O(\epsilon)$ fixed point because the first-order terms of $(1-2X_4/X_8)$ cancel exactly and the next term in the expansion, ϵu, is the same order as u^2. Therefore to determine Δ^* the following equation for $dy/dl=0$ must be used,

$$(\epsilon-2X_4^*u^*)+(\tfrac{3}{2}X_1^*+X_5^*)y^*+2X_9^*u^{*2}=0 \tag{3.17}$$

where

$$X_9^*u^{*2}=\frac{-3(n+2)(7n+16)}{4(n+8)^3}\epsilon^2$$

and (3.18)

$$X_9^*u^{*2}(n=4-g\epsilon)=-\tfrac{11}{96}\epsilon^2+O(\epsilon^3) \ .$$

Thus we find $\Delta^*=C(g)\epsilon$ and $y^*=C(g)\epsilon^3/(3\times 36)$ with $C(g)=(-\frac{11}{16}+g/4)$ where $g\geq 1$. Since the ferroelectric region has $y\geq 0$ the magnitude of g determines whether or not the fixed point is in the ferroelectric region. If $g>\frac{11}{4}$ the fixed point is not in the ferroelectric region. For $g<\frac{11}{4}$ a $y^*\neq 0$ ferroelectric fixed point exists and is characterized by $\Delta^*\sim O(\epsilon)$, $y^*\sim O(\epsilon^3)$, and $u^*\sim O(\epsilon)$. In summary near $\Delta^*=0$ the fixed point is given by $\Delta^*=C(g)\epsilon$, $y^*=C(g)\epsilon^3/(252K_4)$, and $u^*=\epsilon/(48K_4)$. This completes the list of fixed points for $\Delta^*\neq\pm 1$.

We next consider the possibility of fixed points for $\Delta\to\pm 1$. This region is most easily studied after the transformation $p\to p(1-\Delta^2)^{-(d-n-1)/2}$, $\mathbf{x}\to\mathbf{x}$, $\mathbf{x}_N\to(1-\Delta^2)^{-1/2}\mathbf{x}_N$ which changes the free energy to

$$F=\int d\mathbf{X}\left[\frac{1}{2(+1\Delta)}|\nabla\cdot\mathbf{p}|^2+\frac{1}{2(1-\Delta)}|\nabla\cdot\mathbf{p}|^2 + |\nabla_N\mathbf{p}|^2+\bar{w}|\mathbf{p}|^2(\nabla\cdot\mathbf{p})+\bar{u}|\mathbf{p}|^4\right] , \tag{3.19}$$

where $\bar{w}=w/(1-\Delta^2)^{(9-3n)/2}$ and $\bar{u}=u/(1-\Delta^2)^{6-2n}$. Scaling the free energy in this manner changes the propagator to

$$G_{\alpha\beta}(Q)=\frac{T_{\alpha\beta}}{r+(1-\Delta)^{-1}q^2+q_N^2}+\frac{L_{\alpha\beta}}{r+(1+\Delta)^{-1}q^2+q_N^2} \ . \tag{3.20}$$

This is a useful way to express $G_{\alpha\beta}$ because G remains finite in the entire region $(-1\leq\Delta\leq 1)$. Thus the contributions to perturbation theory are small for $\bar{w}$ and $\bar{u}$ small, while they diverge as $\Delta\to\pm 1$ for w, u fixed (and small). Also for $\Delta=1$ $(\Delta=-1)$ we see that the transverse (longitudinal) part of the propagator vanishes so that such fluctuations are strongly suppressed. It will still be assumed that there are only fluctuations with wave vectors $|\mathbf{Q}|<\Lambda$. We remark that it is generally the correct strategy in the renormalization to scale lengths so that the propagator is of order one for $|\mathbf{Q}|=\Lambda$, in so far as possible, and tends to zero (not infinity) when it is not of order one.

The renormalization equations are changed by this transformation because the relative scaling of $\mathbf{x}$ and $\mathbf{x}_N$ is changed and because u and y are changed. In what follows we discuss only the case $n=d$ in which the relative scaling of $\mathbf{x}$ and $\mathbf{x}_N$ is irrelevant. The RG equations are, in the limit $\Delta\to 1$,

$$\frac{d\Delta}{dl}=2(1-\Delta)\bar{y}(\bar{X}_1-\bar{X}_2)+16(1-\Delta)\bar{u}^2(\bar{Y}_1-\bar{Y}_2) , \tag{3.21}$$

$$\frac{d\bar{y}}{dl}=(\epsilon-2\bar{X}_4\bar{u})\bar{y}+6(\bar{X}_1-\bar{X}_2)\bar{y}^2+O(\bar{y}\,\bar{u}^2,\bar{y}^3) , \tag{3.22}$$

and

$$\frac{d\bar{u}}{dl}=\epsilon\bar{u}-\bar{X}_8\bar{u}^2+4(\bar{X}_1-\bar{X}_2)\bar{y}\,\bar{u}+O(\bar{u}^3) , \tag{3.23}$$

where $\bar{X}_i=X_i(1-\Delta^2)^2$ and $\bar{Y}=Y(1-\Delta^2)^3$. Terms which are zero in the limit $\Delta\to 1$, $\bar{u}$, $\bar{y}$ finite have been excluded in $d\bar{y}/dl$ and $d\bar{u}/dl$. The value of $d\Delta/dl$, Eq. (3.21), is clearly zero in this limit. The fixed points $\bar{y}^*$ and $\bar{u}^*$ for $\Delta=1$ are then found by setting the rhs's of Eqs. (3.22) and (3.23) equal to zero. There are four conditions for which the resultant fixed-point equations are solvable: (i) $\bar{y}=\bar{u}=0$, (ii) $\bar{y}=0$ but $\bar{u}\neq 0$ which implies $\bar{u}=\epsilon/\bar{X}_8=\epsilon/(40K_4)$, (iii) $\bar{y}\neq 0$ but $\bar{u}=0$ which implies

$$\bar{y}=-\epsilon/[6(\bar{X}_1-\bar{X}_2)]=-\epsilon/(120K_4) ,$$

and finally (iv) $\bar{y}$ and $\bar{u}$ nonzero which implies

$$\bar{u}=\frac{\epsilon}{(3\bar{X}_8-4\bar{X}_4)}=\frac{-\epsilon}{40K_4}$$

and (3.24)

$$\bar{y}=\frac{\epsilon}{4(\bar{X}_1-\bar{X}_2)}\left[\frac{\bar{X}_8}{(3\bar{X}_8-4\bar{X}_4)}-1\right]=\frac{-\epsilon}{40K_4} \ .$$

TABLE III. The observable fixed points for $d=4-\epsilon$ and $n=4-g\epsilon$ and qualitative nature of the eigenvalues. The stability, that is, the sign of the eigenvalues and the power of ϵ for each eigenvalue, is shown. All constants are positive. For specific numerical values see text.

Fixed point	Δ^*	y^*	u^*	Eigenvalues
Gaussian	$-1\le\Delta\le 1$	0	0	$(0,\epsilon,\epsilon)$
Wilson-Fisher ($g<\frac{11}{4}$)	0	0	$C_u\epsilon$	$(-c_{12}\epsilon^2,-c_{22}\epsilon^2,-\epsilon)$
Wilson-Fisher ($g>\frac{11}{4}$)	0	0	$C_u\epsilon$	$(c'_{12}\epsilon^2,-c'_{22}\epsilon^2,-\epsilon)$
ferroelectric ($\frac{99}{36}<g<\frac{100}{36}$)	$C_\Delta\epsilon$	$C_y\epsilon^3$	$C_u\epsilon$	$(-c_{13}\epsilon^2,-c_{23}\epsilon^2,-\epsilon)$
ferroelectric ($g>\frac{100}{36}$)	$C_\Delta\epsilon$	$C_y\epsilon^3$	$C_u\epsilon$	$((-c_{14}+ic'_{14})\epsilon^2,(-c_{14}-ic'_{14})\epsilon^2,-\epsilon)$
polymeric ($g<\frac{11}{4}$)	$-C_\Delta\epsilon$	$-C_y\epsilon^3$	$C_u\epsilon$	$(c_{15}\epsilon^2,-c_{25}\epsilon^2,-\epsilon)$
polymeric	$-\frac{2}{3}$	$-C_y^P\epsilon$	$C_u^P\epsilon$	$(ic_{16}\epsilon^{3/2}-c'_{16}\epsilon^2,-ic_{16}\epsilon^{3/2}-c'_{16}\epsilon^2,-\epsilon)$
polymeric	$+1$	$-C_y^{P'}\epsilon$	0	$(0,-\epsilon,\epsilon/3)$
ferroelectric	-1	$C_y^F\epsilon$	$C_u\epsilon$	$(-c_{18}\epsilon,-c_{28},\epsilon,c_{38}\epsilon)$

Conditions (i) and (ii) are simply restatements of the Gaussian and the Wilson-Fisher fixed points, respectively, for $\Delta=1$. For condition (iii) a new fixed point is found in the polymeric region. Finally (iv) defines a nonobservable fixed point. However, note that $\bar{y}/\bar{u}=1$ or $\zeta=0$.

The fixed points for $\Delta\to-1$ cannot be determined in the same way. In particular no new fixed points are found for finite $\bar{y}$. The reason is that for the w- (y-) type vertex to contribute to the RG equations there must be longitudinal fluctuations. As the longitudinal fluctuations are suppressed in this limit the effect of y is very small and the contribution to the RG equations is finite even if y is as large as $O(1+\Delta)^2$, as each pair of w vertices requires at least one longitudinal propagator with the associated factor $1+\Delta$. We expect this result to remain true to all orders in perturbation theory. Therefore replacing y and u with $\bar{y}'(1-\Delta)^2$ and $\bar{u}'(1-\Delta)^2$ in Eqs. (3.12)–(3.14) and taking the limit as $\Delta\to-1$ results in

$$\frac{d\Delta}{dl}=-(1+\Delta)\bar{y}'(\bar{X}'_1-\bar{X}'_2)-\tfrac{1}{2}(1+\Delta)^2\bar{u}'^2(\bar{Y}_1-\bar{Y}_2)\ , \qquad (3.25)$$

$$\frac{d\bar{y}'}{dl}=(\epsilon-2\bar{X}_4\bar{u}')\bar{y}'+[3\bar{X}_1+2\bar{X}_5+2(\bar{X}'_1-\bar{X}'_2)]\bar{y}'+O(\bar{y}'^3,\bar{u}'^3)\ , \qquad (3.26)$$

and

$$\frac{d\bar{u}'}{dl}=\epsilon\bar{u}'-\bar{X}_8\bar{u}'^2+[2\bar{X}_1+\bar{X}_6+2(\bar{X}'_1-\bar{X}'_2)]\bar{y}'\bar{u}'+\bar{X}_7\bar{y}'^2+O(\bar{y}'^3,\bar{u}'^3)\ . \qquad (3.27)$$

Again $d\Delta/dl$ is zero in the limit $\Delta\to-1$. The term $[X_1(-1)-X_2(-1)]$ is zero. However,

$$\bar{X}'_1-\bar{X}'_2=[d\bar{X}_1(\Delta)/d\Delta]-[d\bar{X}_2(\Delta)/d\Delta]$$

is nonzero at $\Delta=-1$. Setting the rhs's of these equations equal to zero results in fixed-point equations which again have four possible solutions. There is a trivial solution for $\bar{y}'$ and $\bar{u}'$, and a solution with $\bar{y}'=0$ on the Wilson-Fisher fixed line with $\bar{u}'=\epsilon/136K_4$. The solution for nontrivial $\bar{y}'$ and $\bar{u}'$ is found to be given by a quadratic equation in $\bar{u}'$ which yields solutions for positive and negative $\bar{u}'$. The solution for positive $\bar{u}'$ is given by $\bar{u}'^*=\bar{A}\epsilon$ and $\bar{y}'^*=\bar{B}\epsilon$, where $\bar{A}=0.1385$ and $\bar{B}=0.7894$. In summary there are in addition to the fixed points discussed above four new fixed points in the region $\Delta\to\pm1$: a polymer fixed point, a ferroelectric fixed point, and two nonobservable fixed points ($u<0$). All the fixed points have been displayed in Table III.

C. Stability and exponents

The behavior of the differential equations near the fixed points is now calculated in order to determine their stability. Equations (3.12)–(3.14) are expanded in small displacements near the fixed points with the substitution

$\Delta=\Delta^*+\delta\Delta$, $y=y^*+\delta y$, and $u=u^*+\delta u$. The functions $X_i(\Delta^*+\delta\Delta)$ and $Y_i(\Delta^*+\delta\Delta)$ are expanded in a Taylor series. Terms of linear order are retained, yielding the differential equations

$$\frac{d\delta\Delta}{dl}=[(X_1^*-X_2^*)y^*+(Y_1^*-Y_2^*)u^{*2}+(X_1'^*-X_2'^*)\Delta^*y^*+(Y_1'^*-Y_2'^*)\Delta^*u^{*2}]\delta\Delta$$
$$+[\Delta^*(X_1^*-X_2^*)]\delta y+[2\Delta^*u^*(Y_1^*-Y_2^*)]\delta u\ , \tag{3.28}$$

$$\frac{d\delta y}{dl}=\{-2X_4'^*y^*u^*+[3X_1'^*+2X_5'^*+\tfrac{1}{2}(n-4)(X_1^{*\prime}-X_3^{*\prime})]y^*+X_9'^*y^*u^{*2}\}\delta\Delta$$
$$+\{\epsilon-2X_4^*u^*+2[3X_1^*+2X_5^*+2X_5^*+\tfrac{1}{2}(n-4)(X_1^*-X_3^*)]y^*+X_9^*u^{*2}\}\delta y+(-2X_4^*y^*+2X_9^*y^*u^*)\delta u\ , \tag{3.29}$$

$$\frac{d\delta u}{dl}=\{-X_8'^*u^*+[2X_1'^*+X_6'^*+\tfrac{1}{2}(n-4)(X_1'^*-X_3'^*)]y^*u^*-X_7'^*y^{*2}\}\delta\Delta$$
$$+\{[2X_1^*+X_6^*+\tfrac{1}{2}(n-4)(X_1^*-X_3^*)]u^*-2X_7y^*\}\delta y$$
$$+\{\epsilon-2X_8^*u^*+[2X_1^*+X_6^*+\tfrac{1}{2}(n-4)(X_1^*-X_3^*)]y^*\}\delta u\ , \tag{3.30}$$

where $X_m^*=X_m(\Delta^*)$, $X_m'^*=dX_m/d\Delta\,|_{\Delta=\Delta^*}$.

Since the terms containing r in the Δ, y, and u differential equations are of higher order in ϵ than the terms considered above, they will not be included. The eigenvalue for r can be found by expanding Eq. (3.11) in terms of $r+\delta r$. The term proportional to δr is the exponent ν^{-1},

$$\nu^{-1}=[2-\epsilon+(X_1^*+Y_7^*)y^*+Y_5u^*]\ . \tag{3.31}$$

In determining the flows for small $\delta\Delta$, δy, and δu it is useful to write Eqs. (3.28)–(3.30) in matrix notation. The matrix will be indexed with the following convention: the first, second, and third row (or column) corresponds to Δ, y, and u, respectively.

Substituting $u^*=y^*=0$ in Eqs. (3.28)–(3.30) we immediately find that the Gaussian fixed point is unstable. If either y or u is nonzero then they will increase as $e^{\epsilon l}$ with increasing l. By substituting $u^*=\epsilon/X_8(O)$, $y^*=0$ into the above differential equations, the stability of the Wilson-Fisher (WF) fixed point can be determined. To find the eigenvalues explicitly we assume that near the fixed points the displacements $\delta\Delta$, δy, and δu vary exponentially, i.e., $\delta x_i\sim A_i\exp(\lambda l)$. This leads to the following determinantal equation for λ:

$$R_{\rm WF}(\lambda)=\begin{vmatrix} \left(\lambda+\dfrac{\epsilon^2}{3\times 36}\right) & -\frac{7}{3} & 0 \\ 0 & \left(\lambda+\dfrac{11\epsilon^2}{96}-\dfrac{43}{24\times 48}g\epsilon^3\right) & 0 \\ O(\epsilon) & O(\epsilon) & (\lambda+\epsilon)\end{vmatrix}=0\ . \tag{3.32}$$

Since the only nonzero contribution to this determinant is along the diagonal the eigenvalues to lowest order in ϵ are given by $\lambda=(-\epsilon^2/(3\times 36),\ -(11\epsilon^2/96)+43g\epsilon^3/(24\times 48),\ -\epsilon)$. Therefore the WF fixed point is stable for $g<\frac{11}{4}$, and has one unstable direction for $g>\frac{11}{4}$. The eigenvectors were calculated. In this case, as in the other $\Delta^*\neq\pm 1$ cases, it was found that the relaxation in the u direction was predominantly controlled by the $\lambda=-\epsilon$ eigenvalue and the relaxation in the Δ and y directions by the remaining eigenvalues.

Next we consider the $y^*\neq 0$ fixed points. Substituting $\delta X_i=A_i\exp(\lambda l)$ into the above equations yields the following determinantal equations for λ at the $\Delta=O(\epsilon)$ and the $\Delta=-\frac{2}{3}$ fixed points, respectively:

$$R_0(\lambda)=\begin{vmatrix} \left(\lambda+\dfrac{\epsilon^2}{3\times 36}\right) & -\frac{7}{3} & O(\epsilon^2) \\ \dfrac{-C(g)\epsilon^4}{18\times 21} & \lambda+O(\epsilon^3) & \dfrac{4C(g)\epsilon^3}{21} \\ \dfrac{-\epsilon^2}{48} & O(\epsilon) & (\lambda+\epsilon)\end{vmatrix}=0\ , \tag{3.33}$$

$$R_{-2/3}(\lambda)=\begin{vmatrix} (\lambda-2.045\epsilon^2\times 10^{-5}) & -9.372\times 10^{-2} & -4.094\epsilon^2\times 10^{-3} \\ -3.266\epsilon^3\times 10^{-3} & (\lambda-2.754\epsilon^2) & 2.184\epsilon^2\times 10^{-3} \\ 1.455\epsilon^2 & -0.4424\epsilon & (\lambda+\epsilon)\end{vmatrix}=0\ . \tag{3.34}$$

Equations (3.33) and (3.34) have a solution provided the determinant vanishes. The quantities in the determinant written $O(\epsilon)$ or $O(\epsilon^2)$ can be ignored to lowest order in ϵ. The determinant $R_0(\lambda)=0$ yields

$$\lambda+\epsilon\lambda^2+\frac{\epsilon^3\lambda}{3\times 36}+\frac{C(g)\epsilon^5}{9\times 36}=0\ , \tag{3.35}$$

where the coefficients of each power of λ have been determined only to lowest order in ϵ. Corrections of relative order ϵ are expected. There are three solutions to this cubic equation which are easy to calculate by supposing $\lambda\sim\epsilon^j$. For $j=1$ the λ^3 and the $\epsilon\lambda^2$ terms dominate (the other terms are of higher order in ϵ) so that $\lambda=-\epsilon$. Similarly supposing $j=2$ we find that the λ^2, λ, and λ^0 terms are of $O(\epsilon^5)$ and the λ^3 term is of $O(\epsilon^6)$. Thus the remaining eigenvalues are

$$\lambda_\pm=\epsilon^2 6^{-3}\{-1\pm[1-144C(g)]^{1/2}\}\ . \tag{3.36}$$

In the ferroelectric ($y\geq 0$) region there are three possible types of flows near this fixed point depending on the choice of g. Since both Δ^* and y^* are proportional to $C(g)$, $C(g)$ must be greater than zero ($g\geq\frac{11}{4}$) for the $y^*\neq 0$ fixed point to be a ferroelectric fixed point. The stability of the $y\neq 0$ fixed point is determined from (3.35). For $\frac{99}{36}<g<\frac{100}{36}$ the eigenvalues are of the form $\lambda=(-c_1\epsilon^2,-c_2\epsilon^2,-\epsilon)$ where c_1 and c_2 are small positive constants. Therefore this set of eigenvalues describes a stable fixed point. For $g>\frac{100}{36}$ the eigenvalues are $\lambda=-\epsilon$, $\lambda_\pm=\epsilon^2 6^{-3}(-1\pm c'i)$, where c' is a constant whose value depends on g. Such complex-conjugate eigenvalues with a negative real part imply a stable fixed point with flows which spiral in towards the fixed point. We thus conclude that the fixed point is stable for $g>\frac{11}{4}$. Finally the fixed points coincide and are marginally stable for $g=\frac{11}{4}$. As the Wilson-Fisher fixed point is stable for $g<\frac{11}{4}$ (i.e., one eigenvalue is zero), we conclude that there is a stable ferroelectric fixed point for any g.

Consider the case $1\leq g<\frac{11}{4}$. In this range of g, the quantity $C(g)$ ranges from $-\frac{7}{16}\leq C(g)<0$. Since $C(g)$ is less than zero and both y^* and Δ^* are proportional to $C(g)$, this fixed point occurs in the polymeric region. For $C(g)<0$ the eigenvalues λ which are proportional to $c_\pm=\{-1\pm[1-144C(g)]^{1/2}\}$ of (3.36), are real. They are given by $\lambda=(c_+\epsilon^2,c_-\epsilon^2,-\epsilon)$. Since c_+ is positive and c_- is negative this fixed point near $\Delta=0$ has one unstable eigenvalue and one parameter in addition to temperature (r). Thus it is a tricritical fixed point; it can be reached only by adjusting another parameter in addition to r.

Next consider the $\Delta^*=-\frac{2}{3}$ fixed point. Evaluating $R_{-2/3}(\lambda)$ yields the cubic equation

$$\lambda^3+\epsilon\lambda^2+A\epsilon^3\lambda+A'\epsilon^4=0 \tag{3.37}$$

where A and A' are the appropriate coefactors. As before assuming $\lambda=O(\epsilon)$ gives $\lambda=-\epsilon$. In a first approximation if we suppose that $\lambda=O(\epsilon^{3/2})$ the λ^3 and λ terms of this cubic equation are found to be $O(\epsilon^{9/2})$, and negligible relative to the λ^2 and λ^0 terms which are $O(\epsilon^4)$. However, as A' is positive this yields $\lambda=\pm i\,|A'|^{1/2}\epsilon^{3/2}$, i.e., purely imaginary eigenvalues. In order to determine the stability of the spiral the next-order term in ϵ must be included. This is accomplished by writing $\lambda=\lambda_0+O(\epsilon^2)$. This term of $O(\epsilon^2)$ in λ can be determined entirely from the λ^3 and λ terms in Eq. (3.37) as the corrections to this equation are of relative order in ϵ, e.g., $O(\epsilon^5)$, $O(\lambda^2\epsilon^2)$. Thus the eigenvalues are

$$\lambda_\pm=\pm i\,|A'|^{1/2}\epsilon^{3/2}-(A-A')\epsilon^2/2\ , \tag{3.38}$$

where $|A'|=7.274\times 10^{-4}$ and $(A-A')/2=2.889\times 10^{-3}$. Since the eigenvalues are complex conjugates with a positive real part, they describe a system whose flows begin at the fixed point and spiral outward. Clearly this fixed point with eigenvalues of the form

$$(iO(\epsilon^{3/2})-O(\epsilon^2),-iO(\epsilon^{3/2})-O(\epsilon^2),-\epsilon)$$

is unstable.

Finally we discuss the stability of the observable fixed points for $\Delta\to\pm 1$. For $\Delta\to -1$ a nontrivial ferroelectric fixed point was found with $\bar{y}=\bar{B}\epsilon$ and $\bar{u}=\bar{A}\epsilon$. Using the procedure given above a determinant $R_{-1}(\lambda)$ is found:

$$R_{-1}(\lambda)=\begin{vmatrix}(\lambda+0.420\epsilon) & 0 & 0\\ O(\epsilon) & (\lambda+18.95\epsilon) & -113.7\epsilon\\ O(\epsilon) & 0.4854\epsilon & (\lambda+11.42\epsilon)\end{vmatrix}=0\ . \tag{3.39}$$

Clearly this reduces to the product of $(\lambda+0.420\epsilon)$ and a 2×2 subdeterminant which has the solutions given by $\lambda_+=17.0\epsilon$ and $\lambda_-=-9.47\epsilon$. Thus the $\Delta\to -1$ nontrivial fixed point is unstable. The stability of the order polymer fixed point for $\Delta\to 1$ with $\bar{u}^*=0$ and $\bar{y}^*=-\epsilon/120K_4$ is easily seen by observing that $d\delta\bar{u}/dl=\delta\bar{u}\epsilon/3$ and $d\delta\bar{y}/dl=-\delta\bar{y}\epsilon$. Therefore this fixed point is unstable. The stability of the nonobservable fixed points will not be given.

D. RG flows

The local picture of the trajectories on the parameter space will now be extended to a more global picture. The flow equations (3.12)–(3.14) for the ferroelectric region and polymeric region differ only in that y is of opposite sign. However, this has a significant effect on the flow behavior and $y\geq 0$ and $y\leq 0$ will be discussed separately. However, for any y the $(Y_1-Y_2)u^2$ and X_9yu^2 terms affect the system of equations only when y is small compared to u. If $y\gg u$ then the y^2 term of (3.13) sends the trajectories away from the fixed points and (3.14) toward $u=0$. If $u\gg y$ Eq. (3.13) brings the flows into the fixed-point region. Therefore a region of interest is the region where y and u are small $[O(\epsilon)]$ and comparable and Δ is between ± 1. The change of variables ($y\to\epsilon\tilde{y}$, $y\to\epsilon\tilde{u}$, and $l\to\epsilon\tilde{l}$) gives

$$\frac{d\Delta}{d\tilde{l}}=(X_1-X_2)\Delta\tilde{y}+O(\epsilon)\ , \tag{3.40}$$

$$\frac{d\tilde{y}}{d\tilde{l}}=(1-2X_4\tilde{u})\tilde{y}+[3X_1+2X_5+2(3-d+\tfrac{1}{4}n)(X_1-X_3)]\tilde{y}^2\ , \tag{3.41}$$

$$\frac{d\tilde{u}}{d\tilde{l}}=\tilde{u}-X_8\tilde{u}^2+[2X_1+X_6+(4-\tfrac{3}{2}d+\tfrac{1}{2}n)(X_1-X_3)]\tilde{y}\,\tilde{u}-X_7\tilde{y}^2\ , \tag{3.42}$$

in this region. These three differential equations in $\tilde{l}$ were changed to two differential equations in Δ through the chain rule:

$$d\tilde{u}/d\Delta=d\tilde{u}/d\tilde{l}(d\Delta/d\tilde{l})^{-1}\ ,$$

$$d\tilde{y}/d\Delta=d\tilde{y}/d\tilde{l}(d\Delta/d\tilde{l})^{-1}\ .$$

This can be done unambiguously because $(X_1-X_2)\Delta$ is never zero. These equations were solved numerically.

For $y>0$ three different behaviors were found depending on the initial values of Δ, y, and u: (i) the flows were inward toward $y=0$, (ii) the flows remained on a surface, which we will call the separatrix given by $y[u(1-\Delta)]^{-1}=Z_s(n,\Delta)$, and (iii) the flows were outward toward $y=\infty$ or $u<0$ away from the fixed points. Near $\Delta=-1$ it was found for $n=4$, starting with appropriately chosen y and u values, that the solution extended out away from $y=0$, along a similar path, and then all the way around back to $\Delta=+1$ and $y=0$. This happened for all y and u chosen with a certain ratio. Since this was a surprising result the ratio $Z_s=y[u(1-\Delta)]^{-1}$ was calculated. This was accomplished simply by calculating Z_s for each new Δ, y, and u generated by the integration scheme. We found $Z_s=2$ (which is precisely $\zeta=0$, also found to be of interest in mean-field theory). In other words the line which for $n=4$ separates a region in which there is a second-order transition to a uniform phase and in which there is a first-order transition to a modulated phase is exactly reproduced by the RG to lowest order in ϵ. This can be shown analytically. We have

$$\frac{dZ_s}{d\Delta}=\frac{(\epsilon-2X_4u)+(3X_1+2X_5)y}{\Delta(1-\Delta)u(X_1-X_2)}-Z_s\left[\frac{(\epsilon u-X_8u^2+(2X_1+X_6)yu-X_7y^2)}{y\Delta u(X_1-X_2)}\right]+\frac{Z_s}{(1-\Delta)}\ . \tag{3.43}$$

Substituting $Z_s=2$ into (3.43) we found that for $n=4$, but not for other n, $dZ_s/d\Delta=0$ as an identity in Δ. Thus this ratio completely maps out the region in (Δ,y,u) space for $y>0$ where second-order phase transitions occur. In particular, flows with $y[u(1-\Delta)]^{-1}$ initially less than 2 will remain within the surface and will eventually flow into and terminate at the stable fixed point. Near $\Delta=\pm1$, $\bar{u}$ and $\bar{y}$ are expected to be finite as $d\bar{u}/dl$, $d\bar{y}/dl$, and $d\bar{u}/dl$ are finite. However, this implies $d\Delta/dl\sim(1-\Delta)$. Therefore the flows inside the surface $y/2u(1-\Delta)$ never cross $\Delta=\pm1$. Flows that start outside the surface either escape to infinity or, if $y\le u$, flow to negative u, indicating a first-order transition. Therefore $y[u(1-\Delta)]^{-1}=2+O(\epsilon)$ appears to be a tricritical surface separating systems with second-order transitions from systems with fluctuation-induced first-order transitions. However, it is important to note that there is no tricritical fixed point on this surface. It is easy to see that along the separatrix $d\bar{u}/d\Delta$ is of the form $\epsilon f(\Delta)(1-\Delta)^{-1}-g(\Delta)\bar{u}$ where f and g are finite, smooth functions (except as $\Delta\to-1$). These functions are positive as $\Delta\to1$. Therefore $\bar{u}$ diverges as a power of $\Delta-1$ as $\Delta\to1$. Thus the RG flows are out of the region in which perturbation theory can be applied. See Sec. IV for further discussion.

The invariant nature of the curve $Z_s=2$ for $n=4$ is easy to check at the graphical level. In particular it is easy to see from the graphs of Fig. 8 that to lowest order in u and y

$$\langle p_\alpha(\mathbf{Q})p_\alpha(\mathbf{Q}')p_\beta(\mathbf{Q}'')p_\beta(-\mathbf{Q}-\mathbf{Q}'-\mathbf{Q}'')\rangle_c=-8u+4\frac{y}{1-\Delta}=-4u(2-Z_s) \tag{3.44}$$

provided $\alpha\neq\beta$, $\mathbf{Q}$, $\mathbf{Q}'$, $\mathbf{Q}''$, $Q+\mathbf{Q}'+\mathbf{Q}''$, and $\mathbf{q}+\mathbf{q}'$ are all nonzero and $q_\alpha=q'_\alpha=q''_\beta=q_\beta+q'_\beta+q''_\beta=0$. Thus the statement that $Z_s=2$ is unchanged by the RG is equivalent to the statement that the expectation value of (3.44) is also zero to second order in y and u when $Z_s=2$. This is easy to verify. Consider any graph which contains a u vertex. For each such graph there is a graph in which this vertex has been replaced by a pair of w vertices connected by a single longitudinal propagator

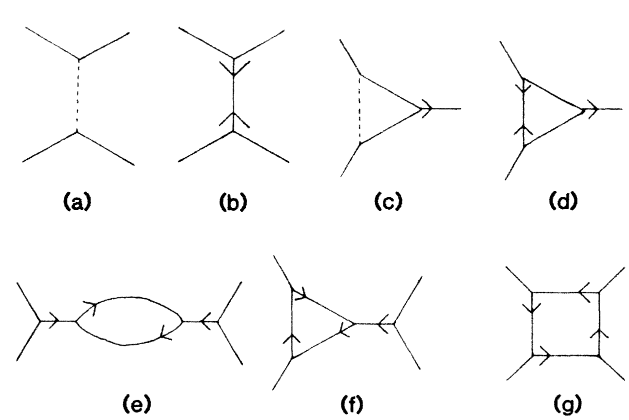

FIG. 8. The Feynman diagrams which contribute to the renormalized value of $Z_s=2$. (a) and (b) are the contributions to lowest order; (c) and (d) are examples of graphs which cancel by simple arguments when $n=d$, $Z_s=2$. Graphs (e), (f), and (g) cancel, but not by these simple arguments, when $n=d$, $Z_s=2$.

in the configuration shown in Fig. 8(b). If these graphs are counted prior to considering all topologically equivalent graphs it is clear that there is exactly one graph with this configuration of w vertices for each graph with a u-type vertex. As the u vertex contributes a factor $-u$ and this configuration of w vertices contributes a factor $2y(1-\Delta)^{-1}$ these pairs of graphs cancel when $Z_s=2$. In consequence when $Z_s=2$ it is only necessary to consider graphs which contain neither u vertices nor pairs of w vertices in the configuration of Fig. 8(b). This decreases very appreciably the number of graphs which must be considered. In fact there are only three such graphs contributing to the expectation of Eq. (3.44), shown in Fig. 8. These are easily evaluated, directly or by reference to the work of Blankschtein *et al.*,[8] and are seen to cancel each other. Thus we have verified this (somewhat surprising) result. This gives us considerable confidence in the (rather complex) calculation required to calculate the renormalization-group equations.

It is also instructive to find the separatrix for $n \neq d$. For $n \neq d$ the surface is given by $Z_s = Z_s(n,\Delta)$. We note that the argument given above in the case $n=d=4$ fails when $n \neq 4$; in fact when $n \neq 4$, Z_s is no longer constant. However, it is easy to see that $dZ_s/dl=0$ when $\Delta=1$ and $Z_s=2$, independent of n. Therefore, as $d\Delta/dl=0$ when $\Delta \rightarrow 1$ ($\bar{u},\bar{y}$ finite) the separatrix must end at $Z_s(n,\Delta=1)=2$. The values of Z_s for $n \neq 4$ must be found numerically by integrating Eq. (3.43). For $n=d=4$, $Z_s=2$ is a straight line and for $n=3$, Z_s is roughly constant and close to but slightly greater than 2. Around $n=2.5$ the quantity Z_s and the flow equations change dramatically in that for $\Delta<0$ the flows become directed outwards. Figure 9 shows how the behavior of the flows changes as n is varied.

Flows originating outside the separatrix flow away from the fixed point. Any flow which begins within the separatrix described above will stay inside this surface. Such flows flow eventually to small values of $\tilde{y}$. This motivates the study of the flow equation for small $\tilde{y}$. The $\tilde{y}^2$ term in (3.41) and (3.42) and the $\tilde{y}\tilde{u}$ term in (3.42) can then be ignored. This approximation leads to an analytic solution for $\tilde{u}$ with

$$\tilde{u} = \frac{B'e^l}{(1+B'X_8e^l)} \sim \frac{1}{X_8} . \tag{3.45}$$

Then assuming $\tilde{u}$ is close to X_8^{-1} we find

$$\tilde{y} = \frac{Be^l}{(1+X_8e^l)^{X_4/X_8}} \sim \frac{Be^{(X_4-2X_8)l/X_8}}{X_8^{X_4/X_8}} , \tag{3.46}$$

where B and B' are constants and the second quantities indicated above in (3.45) and (3.46) are the asymptotic forms. The solution for y in this region shows that the flows are inward toward the $y=0$ plane for $(1-2X_4/X_8)<0$ and outward for $(1-2X_4/X_8)>0$. Thus these (incomplete) equations have a stable fixed line for $u=\epsilon/X_8$, $y=0$, $(1-2X_4/X_8)<0$. Of course for the full equations this is no longer a fixed line, although because the term which has been ignored in the derivation

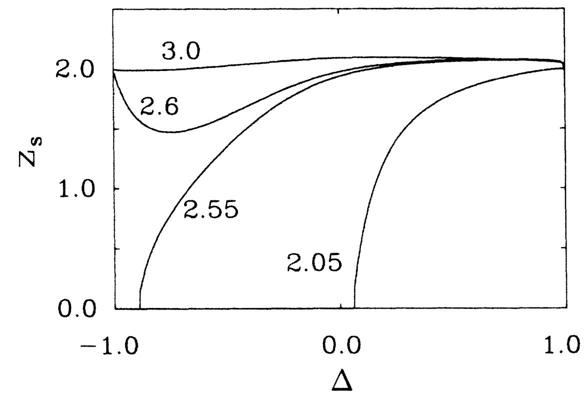

FIG. 9. Plot of separatrix $Z_s(n,\Delta)$ for $n=3$, 2.6, 2.55, and 2.05 in the ferroelectric region. The straight line $Z_s(4,\Delta)=2$ is not shown.

of this quasifixed line is numerically very small (in more than two spatial dimensions), in actual experiments a point on this fixed line may control the behavior of the system except for temperatures unattainably close to the transition temperature. Because of this it is interesting to calculate the critical behavior along this line. The exponent $\nu^{-1}=2-\epsilon(1+Y_5/X_8)$ was calculated along the quasifixed line $u^*=\epsilon/X_8$ with $y=0$, for $n=3$ ($\epsilon=1$). It was found that ν^{-1} was essentially constant ($\nu^{-1}\simeq 1.5$) in the interval $-1 \leq \Delta \leq 1$. The minimum value of $\nu^{-1} \sim 1.45$ occurred at $\Delta=0$ and the maximum $\nu^{-1} \sim 1.53$ at $\Delta=1$.

We now discuss the behavior of the RG flows after they come close to this quasifixed line. Solution (3.45) simply restates that the flows for u are inward toward the fixed line in a region of Δ's. So starting in the region with y small but nonzero and $(1-2X_4/X_8)<0$ the trajectories flow inward toward $y=0$ and the quasifixed line given by $u=\epsilon/X_8$. Of course this line, $y=0$ and $u=\epsilon/X_8$, is not actually a fixed line because of the u^2 term in $d\Delta/dl$. As y is very small the flow equations for Δ and u are

$$\frac{d\Delta}{dl} = \Delta(Y_1-Y_2)u^2 \tag{3.47}$$

and

$$\frac{du}{dl} = u - X_8u^2 . \tag{3.48}$$

Since $\Delta(Y_1-Y_2)$ is positive for $\Delta<0$ and negative for $\Delta>0$ this quantity will always take the flows toward $\Delta=0$.

We must also account for the behavior of y in the region where y is small but nonzero and $u \sim \epsilon$. This will be done by calculating the function $y=y(\Delta)$ for $\Delta<0$. To find this function (3.13) is divided by (3.12) and only the leading terms in y are retained yielding

$$\frac{dy}{d\Delta} = \frac{(\epsilon-2X_4u)y}{\Delta(Y_1-Y_2)u^2} . \tag{3.49}$$

Substituting $u=\epsilon/X_8$ we find

$$y=\exp\left[\frac{1}{\epsilon}[G(\Delta)-G(\Delta_0)]\right],$$

where (3.50)

$$G(\Delta)=\int d\Delta\left[1-\frac{2X_4}{X_8}\right]\frac{X_8^2}{\Delta(Y_1-Y_2)}$$

and $G(\Delta_0)$ is a constant of integration. The function $G(\Delta)$ was evaluated numerically for $n=4$ and is shown in Fig. 10. To order ϵ, Δ_0 is the value of Δ at which the flows of Eqs. (3.40)–(3.42) reach the quasifixed line. Thus it is found that if the flows have $\Delta_0<-0.77$ or $\Delta_0>0$, the flows will flow all the way into the Wilson-Fisher fixed point along the quasifixed line. If $-0.77<\Delta_0<0$ the flows will flow along the quasifixed line until $[G(\Delta)-G(\Delta_0)]\sim O(\epsilon)$ when y grows rapidly. The flows then follow Eqs. (3.40)–(3.42) and flow into the $\Delta>0$ region and to the quasifixed line. They then flow in again along this line to the Wilson-Fisher fixed point. Note, however, that when $y=0$ the flows will follow the fixed line all the way to the Wilson-Fisher fixed point $u^*=\epsilon/48K_4$.

The flow behavior near the $\Delta\sim\epsilon$ fixed point for $n\neq4$ (or, more properly when the $y^*\neq0$ fixed point does not coincide with the Wilson-Fisher fixed point) is also described by the function $G(n,\Delta)$. The function $[1-2X_4(n,\Delta)/X_8(n,\Delta)]$ is nonzero at $\Delta=0$ except for $n=4$ (see Fig. 7). It follows that $G(n\neq4,\Delta=0)\neq0$. Using the expansion of Eq. (3.16) it is found, to leading order in Δ (near $\Delta=0$), that

$$G(n=4-g\epsilon,\Delta)=36\epsilon^{-1}(\Delta-\Delta^*\ln|\Delta/\Delta^*|)\ .$$

Since $G(n,\Delta)$ has a logarithmic divergence at $\Delta=0$ for $\Delta^*\neq0$, the nature of the flows reaching the quasifixed line in the ferroelectric region depends on the sign of Δ^*. If $\Delta^*<0$ then $G(n,\Delta)\to-\infty$ as $\Delta\to0$ and

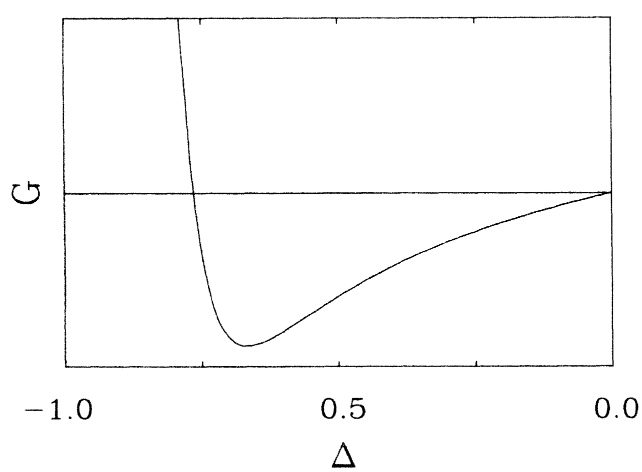

FIG. 10. Plot of the function $G(n=4,\Delta)$ for $-1\leq\Delta\leq0$. The point where $G(\Delta)$ crosses the Δ axis is $\Delta\simeq-0.77$.

$$y\sim\exp\{\epsilon^{-1}[G(n,\Delta)-G(n,\Delta_0)]\}$$

so the flows are inward, all the way to the Wilson-Fisher fixed point. However, for $\Delta^*>0$, the flows originating with $\Delta<0$ cannot flow directly through $\Delta=0$ to the $\Delta^*=C(g)\epsilon$, $y=C(g)\epsilon^3/252K_4$ fixed point. This is because as $\Delta\to0^-$,

$$[G(n,\Delta)-G(\Delta_0)]\to0(\epsilon)\ ,$$

and

$$y\sim\exp\{\epsilon^{-1}[G(n,\Delta)-G(\Delta_0)]\}$$

grows rapidly. However, in the ferroelectric region, flows beginning with $y[u(1-\Delta)]^{-1}<Z_s$ remain in this region, as we have shown above. When $G(\Delta)-G(\Delta_0)=O(\epsilon)$, y increases, the flows follow Eqs. (3.40)–(3.42) and cross $\Delta=0$ and for some $\Delta>\Delta^*$ flow inward and reach the quasifixed line. As the function $G(n,\Delta)$ is minimum at $\Delta=\Delta^*$ such flows, or any flows which reach the quasifixed line for $\Delta>\Delta^*$ first flow inward along it. However, provided Δ_0 is not too close to Δ^* for some $\Delta<\Delta^*$ they flow out of this region when $G(n,\Delta)-G(n,\Delta_0)=O(\epsilon)$ and flow via Eqs. (3.40)–(3.42) which takes the flows increasing in Δ $[d\Delta/dl=\Delta y(X_1-X_2)>0]$, and towards $y=0$ again. Since the flow lines never cross, they are trapped and flow inward within the previous flow lines and repeat this cyclic process, and spiral into the fixed point.

In the polymeric region ($y<0$) the surface Z_s outlined above is very different. The flow equation (3.12)–(3.14) for this region will be discussed only for $n=d$. Since $y<0$, $d\Delta/dl=\Delta\tilde{y}(X_1-X_2)<0$ for all Δ $[\Delta(X_1-X_2)$ is always positive], and the flows have Δ decreasing unless $\tilde{y}$ is very small. In addition if y and u are $O(\epsilon)$, Eqs. (3.40)–(3.42) can be used. When $\tilde{y}$ becomes significant the $|\tilde{y}|^2$ term of Eq. (3.41) becomes dominant and $\tilde{y}$ grows rapidly. For $\tilde{y}\sim\tilde{u}$, the terms $\tilde{y}\,\tilde{u}$ and $\tilde{y}^2$ of $d\tilde{u}/dl$ are both negative which takes $\tilde{u}$ quickly to zero unless both $\tilde{y}$ and $\tilde{u}\ll1$. Therefore $\tilde{y}$ must grow faster than $\tilde{u}$ tends to zero to reach the fixed point region.

There are three different regions with $-1\leq\Delta\leq1$, $\tilde{y}<0$, and $\tilde{u}>0$, where second-order behavior occurs. The largest region extending from $0\leq\Delta\leq1$ was determined by numerical integration. It was found that flows beginning within a line $Z_s'\sim1$ $\{Z_s'=y/[u(1-\Delta)]\}$, flow into $\tilde{y}=0$ and to the Wilson-Fisher fixed point. There is also a very small region which extends from $\Delta=0$ to $\Delta\simeq-0.4$ with $Z_s'\sim e^{-O(1/\epsilon)}$. In this region the flows follow Eqs. (3.47)–(3.50) towards $\Delta=0$. If the initial value of y is small enough the flows have y less than the tricritical value at the tricritical polymeric fixed point and will tend to the Wilson-Fisher fixed point. Finally there is an interesting region extending from $\Delta\simeq-0.4$ to $\Delta=-1$ with $Z_s'\sim1$. This is the region which contains the $\Delta^*=-\frac{2}{3}$ fixed point. Because of the unstable nature of this fixed point, (i.e., the flows spiral outward) flows originating in this region can either flow inwards to $\tilde{y}=0$ and along the quasifixed line to the fixed point or outwards and into negative $\tilde{u}$. This behavior is schematically shown in Fig. 11.

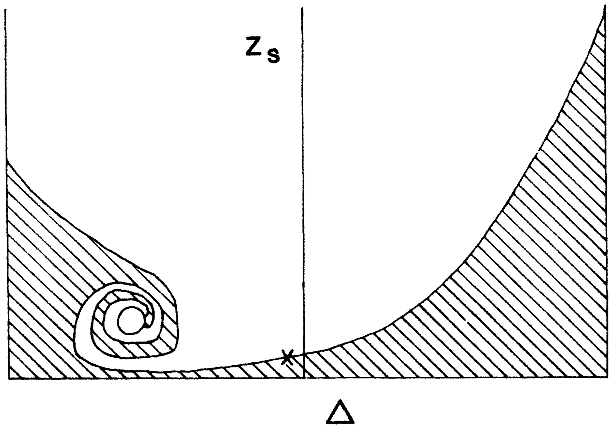

FIG. 11. Schematic representation of the polymeric ($y<0$) region for $-1\leq\Delta\leq 1$. The regions enclosed by $Z_s(n=4,\Delta)$ are (a) $Z_s'=O(1)$ ($0\leq\Delta\leq 1$), (b) $Z_s'=e^{-O(1/\epsilon)}$ ($-0.4\lesssim\Delta<0$), and (c) $Z_s'=O(1)$ ($-1\leq\Delta\lesssim-0.4$). The function Z_s' is minimum at $\Delta=-\frac{2}{3}$. The unstable $\Delta^*=-\frac{2}{3}$ fixed point is indicated by an open circle and the tricritical $\Delta^*=C(g)\epsilon$ [$C(g)<0$] fixed point is indicated by $\times$. All flows originating in the shaded region eventually reach the stable, Wilson-Fisher fixed point. Flows which originate in the unshaded region flow away.

This last region can be best understood by considering the function $G(\Delta)$. As we have shown above, the flows originating with $\Delta_0<-0.77$ and $y\ll 1$ flow along the quasifixed line to the Wilson-Fisher fixed point. Therefore any point which flows following Eqs. (3.40)–(3.42) to the quasifixed line ($y\to 0$) with $-1>\Delta>-0.77$ flows to the Wilson-Fisher fixed point. Some flows originating with $\Delta<-0.4$ and with $y[u(1-\Delta)]^{-1}<Z_s'$ flow to this part of the quasifixed line. Other flows, however, will reach another part of the quasifixed line. These flows flow along the quasifixed line until $G(\Delta')=G(\Delta_0)$, when they are once again controlled by Eqs. (3.40)–(3.42). If $\Delta'>-0.4$ the resultant flow is to a first-order region; if $\Delta'<-0.4$ the resultant flow again reaches the quasifixed line, with a more negative value of Δ_0. In the shaded region this cycle continues until $\Delta_0<-0.77$ is reached when the flow reaches all the way to the fixed point. Similarly the flows beginning in the unshaded region go through this same cycle but flow out of this region before they flow to $\Delta_0<-0.77$. Clearly there must be an unstable region which flows to y small and $\Delta<-0.77$ because flow lines never cross. This spiral behavior matches smoothly on to the spiral behavior around the unstable fixed point.

IV. DISCUSSION

In Sec. II we have discussed mean-field–theory calculations of the disordered, uniform, and modulated phases of the free energy (2.6). In Sec. III we discussed the RG flows for the same model. In this section we review and combine the results of these two sections and discuss the results which would be expected in actual systems.

In Sec. III we found a separatrix for $-1\leq\Delta\leq 1$ given by $\zeta=O(\epsilon)$ for $n=d=4-\epsilon$ and ζ of order one, but tending to $O(\epsilon)$ as $\Delta\to 1$ for $n<d=4-\epsilon$. Flows with ζ initially more than the separatrix value remain within this region under the RG flows, except that if the system is initially too close to this separatrix the RG flows flow out of the region in which perturbation theory can be applied. Therefore all systems for which the initial "bare" parameters have ζ larger than, but not too close to, the separatrix, will flow to a stable fixed point with small w (large, positive ζ). In Sec. II we showed that for positive ζ there are, within mean-field theory, two possible phases separated by a second-order transition; the disordered and the uniform ordered phase. Therefore it is expected that such a system will have a second-order transition between a disordered and a uniform state, as a function of the temperature (r). The RG flows are very slow in part of this region and, in fact it is expected that for most initial values of the parameters the flow will reach a quasifixed line rather than a fixed point for any experimentally feasible approach to the critical temperature. Thus the transition is better described in terms of effective exponents than actual exponents. However, the effective value for ν, given Sec. III C, is essentially constant. It is interesting to note that the actual flows near the fixed points are, in some cases, predicted to be helical, resulting in (slowly) oscillating corrections to the asymptotic critical behavior. Also, the quasifixed-line behavior (slowly changing critical behavior) may, very close to the critical point, revert to quickly changing critical behavior. This occurs as the flows approach the helical fixed points.

On the other hand flows which start outside, but again not to close to, the separatrix are carried by the RG flows away from this surface and ζ decreases to -1. As has been shown in Sec. II A and elsewhere[8] $\bar{F}$ ceases to be bounded from below for some $\zeta=\zeta_t$ with (for $2\leq n<4$) $0>\zeta_t>-1$. We conclude that systems with initial parameters in this region of parameter space will have a transition between the disordered state and a modulated state. This transition is strongly first order if the initial value of ζ is sufficiently negative or weakly (fluctuation-induced) first order if the initial value of ζ is not so negative. Thus systems in which fluctuations are important have first-order transitions from the disordered to the modulated state (as a function of the temperature r), for most of the range of initial parameters, unlike the second-order transitions found in the mean-field treatment of Sec. II C. The nature of the modulated state when the transition is strongly first order will depend on the nature of the higher-order terms, which have not been discussed. In the case of fluctuation-induced phase transitions (with initial values of ζ not to close to the mean-field value of ζ_t) we expect that the modulated phase is correctly given by the texture which minimizes $\bar{F}$ for ζ slightly less negative than ζ_t. This state may be the phase discussed by Blankschtein *et al.*,[8] for $n=3$, a body-centered-cubic (bcc) phase and for $n=2$ either a linear modulated phase or a hexagonal phase.

As the temperature decreases from the transition temperature it is appropriate to stop the RG when $r(l)$ is of order 1. Thus the effective value of $-\zeta$ for which mean-field theory should be applied decreases with decreasing temperature. This has interesting consequences. In particular we have shown in Sec. II C that the modulated phase, for $n>2$ and small $-\zeta$, is expected to be a close-packed structure. This is, for $n=3$, inconsistent with a bcc phase. It is also difficult from the point of view of the harmonic expansion, which is expected to be legitimate for large, negative ζ, to see that either of the close-packed lattices, e.g., face-centered cubic (fcc) or hexagonal close packed (hcp), should have lower free energies than the bcc phase previously studied, as the decrease in free energy in the harmonic expansion comes mostly from triplets of the smallest reciprocal-lattice vectors which add to zero. There are no such triplets in the reciprocal lattice of the fcc lattice, and fewer in the reciprocal lattice of the hcp lattice than the bcc lattice. This suggests that, for $n=3$ and small enough initial values of $|\zeta|$, there are two modulated phases with different symmetries and a transition between them as a function of the temperature (r) or the initial value of ζ.

In addition the effective value of ζ may change sign as a function of temperature (see Fig. 1), resulting in a transition between the uniform and modulated phases. As discussed in Sec. II C this transition will be affected by fluctuations very (exponentially) close to the transition. There may also be new phases which appear due to dangerous irrelevant variables for sufficiently small ζ, again as discussed in Sec. II C. We have not discussed the effects of the dangerous irrelevant variables quantitatively in this paper; we have only demonstrated their existence.

The question of what will happen to systems with initial parameters very near the separatrix is more complicated. In particular we did not find a tricritical fixed point on the separatrix and it is easy to see that, to the order we have calculated, the flows along the separatrix flow out of the region in which perturbation theory can be applied. Usually such a flow in the $d=4-\epsilon$ RG is interpreted as implying a first-order transition. However, we do not believe that this is the correct interpretation in this case. Rather we speculate that the situation is rather like that in two-dimensional point-defect-mediated transitions,[20,21] e.g., the $2-d$ X-Y model and $2-d$ melting. It is easy to see that, provided the system is initially in the region in which perturbation theory can be applied, then perturbation theory can still be applied for the flows along the separatrix until Δ is close to 1. As the separatrix tends to $\zeta=O(\epsilon)$ for any n as $\Delta\rightarrow 1$ we find that the flows will flow out of the region in which perturbation theory can be applied only when ζ is small. We have shown in Sec. II D that for ζ small enough the fluctuations associated with localized defects (which have not been included in our momentum-space RG treatment) become important and are expected to result in a disordered state. Thus it seems reasonable that the momentum-space RG should be stopped when the value of the perturbation parameters is of order one $(\bar{y}\sim\bar{u}\sim 1)$. When this is the case the core energy of local point defects, which is inversely proportional to these parameters, is also of order one. In addition, the core energies of a number of higher-dimensional (line, area etc.), defects is of order one per unit size, in units in which the current cell size is one. Therefore a correct treatment of the fluctuations requires treatment of these fluctuations. Such a treatment is complicated. The relative energies of these various defects depends on the values of dangerous irrelevant variables, as discussed in Sec. II D, and it is easy to verify that these variables are still finite when perturbation theory ceases to be applicable. In addition there are interactions between these defects because low-energy defects are only consistent with certain order-parameter textures so that there must be nontrivial textures between defects. Because there are important new fluctuations in this region we speculate that the disordered-ordered state transition temperature will be strongly suppressed in this region. However, we have not performed such a calculation and, in consequence, can not verify this speculation. Nor have we deduced the nature of the transition in this region.

These flows near the separatrix are particularly relevant to the discussion of the uniform phase to modulated phase transition for $n=d$ (or for $n<d$ in the limit $\Delta\rightarrow 1$). We have shown that, within mean-field theory, the uniform-modulated phase transition occurs at $\zeta=0$. This transition was shown, within mean-field theory, to be a higher-order transition with dimension-dependent exponents. It was also seen that dangerous irrelevant variables were expected to effect the transition and that fluctuations would be important close enough to the transition. However, for $n=d$ or as $\Delta\rightarrow 1$ the mean-field transition coincides with the RG separatrix, at least to within corrections of order ϵ. Because of this coincidence and because we have shown that the flows close to the separatrix tend to a region which has not been treated theoretically we cannot, on the basis of the treatment in this paper predict the nature of the uniform-modulated phase transition. However, given that, as discussed in Sec. II D, dangerous irrelevant variables can effect the nature of the modulated phase we speculate that there are several different modulated phases with transitions between them as ζ, r, or other variables are varied.

It is important to note that crystalline ferroelectrics are not well described by the free energy of Eq. (2.1) with $m=2$. Even in cubic crystals two other terms are allowed in F_4. The extent to which the results of this paper will be changed by the effects of these terms is unknown. It should, however, be noted that screened, chiral smectic C films and screened, chiral but untwisted bulk smectic C ferroelectrics are expected to be well described by this free energy.

Finally we remark that the system described in this paper is a simple (at least in the statement of the problem) example of a wide class of ferrodisplacive transitions which have symmetries which allow for terms of the form $p^2\partial p$. We anticipate that the techniques discussed in this paper are more widely applicable.

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