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Brief Reports

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Stability of commensurate phases near the critical temperature: A renormalization-group calculation

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The phase diagram of a modulated system in a field which changes the periodicity is investigated near the critical temperature. For certain values of the field, the system can gain energy by locking into phases where the wave vector is commensurable with the reciprocal-lattice vectors. The widths, Δ_k, of these phases are calculated by renormalization-group theory in $4-\epsilon$ dimensions. We find $\Delta_k \sim [(T_c-T)/T]^{\xi_k}$, with

$$\xi_k = \frac{1}{2}(k-1)\left(1+\frac{2k^2-4k+3}{10(k-1)}\epsilon - \frac{8k^3-20k^2+6k+1}{100(k-1)}\epsilon^2\right) ,$$

where $2k$ is the order of the commensurability. Near T_c, the wave vector locks into every single commensurate value as the field is varied, thus generating a "devil's staircase"-like behavior.

I. INTRODUCTION

Periodically modulated structures are very common in solid-state physics.[1] The ordered structure may be a spin-density wave or a helical magnetic structure as found in many rare-earth systems, a charge-density wave as found in layered compounds such as $TaSe_2$ and in quasi-one-dimensional conductors such as tetrathiofulvalene-tetracyanoquinodimethane (TTF-TCNQ), or a "mass-density" wave as found in rare-gas monolayers absorbed on graphite and in graphite intercalation compounds.

Generally, the periodic structure can gain "umklapp" energy by locking into phases which are commensurate with the lattice, i.e., the wave vector $\vec{q}_k$ can be written as a rational fraction of the reciprocal-lattice vectors.[2–8] This may give rise to phase diagrams including an *infinity* of commensurate phases which may or may not be separated by an infinity of incommensurate phases.[4–8] In particular, mean-field theory predicts that if the system is subjected to a field which changes the periodicity, the wave vector will lock into every single commensurate value it passes, at least when the temperature is close enough to the critical temperature, T_c. The widths of the commensurate phases vanish as power laws as $T\rightarrow T_c$.[4–6]

In this paper we investigate the effects of fluctuations by means of renormalization-group calculations in $4-\epsilon$ dimensions. We find that the exponents governing the widths of the commensurate are modified, but the mean-field phase diagram essentially remains valid.

The order parameter describing a periodic structure is generally complex, $M_{\vec{q}} = X_{\vec{q}} + iY_{\vec{q}}$, and the phase transition thus belongs to the XY universality class.[9] We shall consider a system with wave vector $\vec{q}=(0,0,q_z)$. In mean-field theory, in the vicinity of the commensurate phase with $\vec{q}=\vec{q}_k=(0,0,\pi/k)$ the free energy has the following form:

$$F_{\vec{q}} = -\frac{1}{2}[r+(q_z-\delta)^2]M_{\vec{q}}M_{-\vec{q}} + \sum_K [u_{2k}(M_{\vec{q}}M_{-\vec{q}})^k + v_{2k}(M_{\vec{q}}^{2k}+M_{\vec{q}}^{2k})\delta(\vec{q}-\vec{q}_k)] \quad , \qquad (1.1)$$

where r, u_{2k}, and v_{2k} are phenomenological expansion coefficients. When $\delta = v_{2k}=0$ this is the usual XY model describing a transition into an ordered phase with $M_{\vec{q}_k}\neq 0$. When $\delta\neq 0$ this remains an XY

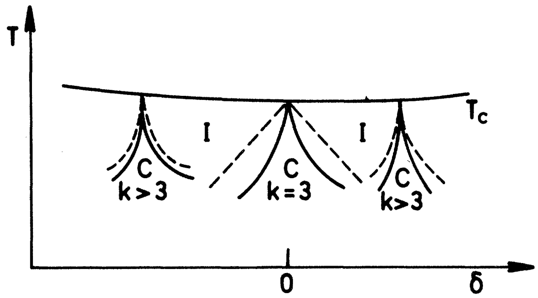

FIG. 1. Schematic phase diagram for periodic structure on a lattice near T_c. The broken line shows the mean-field behavior.

model, but into a phase with $M_{\vec{q}} \neq 0$, $\vec{q} = \vec{q}_k + (0,0,\delta)$. When $v_{2k} \neq 0$, mean-field theory gives a transition into an incommensurate phase[4–6] when the energy involved in forming a domain wall, or soliton, in the commensurate phase becomes negative. This energy (per unit length) is

$$E_S = \left(\frac{4(v_{2k}|M_{\vec{q}}^{2k}|)^{1/2}}{\pi} - \delta|M_{\vec{q}}| \right) , \tag{1.2}$$

so the transition takes place at

$$\delta|M_{\vec{q}}| \sim (|M_{\vec{q}}|^{2k} v_{2k})^{1/2} . \tag{1.3}$$

Near T_c, $|M_{\vec{q}}| \sim t^{1/2}$ so in this limit the borderline value is given by

$$\delta_c \sim \Delta_k \sim |t|^{\xi_{\rm MF}} , \quad \xi_{\rm MF} = \frac{k-1}{2} , \tag{1.4}$$

where $t = (T - T_c)/T_c$. At the critical value of δ, the commensurate phase becomes unstable with respect to soliton formation.[4] The resulting mean-field phase diagram is indicated in Fig. 1. The upper curve separates the disordered phase from the incommensurate one (with $\vec{q}_0$ varying continuously along the line). The lower curves bound commensurate phases with the wave vectors $\vec{q}_k$. The shapes of these curves are given in mean-field theory by Eq. (1.4).

II. EFFECTS OF FLUCTUATIONS

We now concentrate on the vicinity of the commensurate phase in which $\vec{q} = \vec{q}_k$. In this phase the important fluctuations are those with wave vectors $\vec{q} = \vec{q}_k + \vec{p}$, with small values of $\vec{p}$. With a cutoff $|\vec{p}| < \Lambda$, and choosing $\delta = v_{2k} = 0$, the appropriate Landau-Ginzburg-Wilson Hamiltonian takes the form

$$H = -\frac{1}{2} \int_{\vec{p}} (r + p^2) S_{\vec{p}} S_{-\vec{p}} + u_4 \int_{\vec{p}_1} \int_{\vec{p}_2} \int_{\vec{p}_3} S^*_{\vec{p}_1} S_{\vec{p}_2} S_{\vec{p}_3} S^*_{-\vec{p}_1 - \vec{p}_2 - \vec{p}_3} + \text{higher-order terms} , \tag{2.1}$$

where

$$S_{\vec{p}} = M_{\vec{q}_k + \vec{p}} . \tag{2.2}$$

This is an XY model for which the critical exponents can be calculated in $d = 4 - \epsilon$ dimensions.[10] We now switch on a nonzero δ, while v_{2k} remains zero. Clearly, the result is a shift of $\vec{q}$ from $\vec{q}_k$ to $\vec{q}_k + (0,0,\delta)$, with the same XY exponents. The order parameter thus becomes $M_{\vec{q}}$ for any infinitesimal value of δ. This result will change once the umklapp term v_{2k} is introduced, since this term stabilizes the commensurate phase.

For small δ and v_{2k} we expect all the critical properties in the commensurate phase to be described by the scaling properties of the XY model. Thus, we expect the free energy to have the form

$$F(t, \delta, v_{2k}) = |t|^{2-\alpha} f(\delta|t|^{-\nu}, v_{2k}|t|^{-\lambda_k \nu}) , \tag{2.3}$$

where $t = (T - T_c)/T_c$, with T_c being the transition temperature into the commensurate phase, while α and ν are the specific-heat and the correlation-length exponents of the XY model, and λ_k is the scaling exponent for the field v_{2k}. The scaling of δ as $|t|^{-\nu}$ simply follows from the fact that δ is a "momentum," i.e., an inverse length.

The function F is expected to be singular at the commensurate-incommensurate transition. This singularity must arise as a singular line for the scaling function $f(x,y)$, i.e., $x_c = X(y_c)$. Since we expect the transition to occur at $\delta = 0$ when $v_{2k} = 0$, this function must have the form[11]

$$x_c = y_c^{\theta} . \tag{2.4}$$

Substituting $x_c = \Delta_k |t_c|^{-\nu}$ and $y_c = v_{2k}|t_c|^{-\lambda_k \nu}$ this yields

$$\Delta_k = v_{2k}^{\theta} |t_c|^{\nu(1-\theta\lambda_k)} . \tag{2.5}$$

The explicit value of θ must be determined by a calculation. We shall see that by iterating the renormalization group and matching with mean-field theory one finds $\theta = \frac{1}{2}$. The leading operator coupled to v_{2k} is easily identified as the appropriate "cubic" operator $(X_{q_k}^{2k} + Y_{q_k}^{2k})$, and thus v_{2k} is the same as the $g_{0,2k}$ defined by Houghton and Wegner.[12] They find

$$\lambda_k = 4 - 2k + \epsilon[k - 1 - k(2k-1)/5] + \frac{\epsilon^2}{50}[2k(2k-1)(2k-3) - k] . \tag{2.6}$$

Combining all of this with ε-expansion results for ν,[10]

$$2\nu = 1 + \frac{\epsilon}{5} + \frac{11}{100}\epsilon^2 ,$$

we find that

$$\Delta_k = v_{2k}^{1/2} |t_c|^{\xi_k}$$

with

$$\xi_k = \frac{1}{2}(k-1)\left[1 + \frac{2k^2-4k+3}{10(k-1)}\epsilon - \frac{8k^3-20k^2+6k+1}{100(k-1)}\epsilon^2\right] . \quad (2.7)$$

This is the main result of our calculations. It implies a modified shape for the curves bounding the commensurate phases as indicated in Fig. 1.

To obtain the result $\theta = \frac{1}{2}$ we start with the Hamiltonian (2.1), including the umklapp term with coefficient v_{2k}, and perform l^* iterations of the renormalization group, each time increasing the length scale by a factor e, until we have $t(l^*) = -\frac{1}{2}$ (see Rudnick and Nelson, Ref. 13). Since we are in the ordered phase, we first shift the order parameter

$$S_{\vec{p}=0} \rightarrow S_{\vec{p}=0} + M . \quad (2.8)$$

After l^* interations, u_4 practically reaches its XY-model fixed-point value, while the parameters M, δ, and v_{2k} rescale as

$$t(l) = te^{l/\nu}, \quad M(l) = Me^{(1-\epsilon/2)l} ,$$
$$\delta(l) = \delta e^{-l}, \quad v_{2k}(l) = v_{2k}e^{\lambda_k l} . \quad (2.9)$$

At l^*, all the important fluctuations have been eliminated and we can use mean-field theory to determine the line on which the commensurate phase becomes unstable. As discussed in the introduction this happens when Eq. (1.3) is obeyed, i.e., when

$$\delta(l) \sim v_{2k}(l)^{1/2}|M(l)|^{k-1} . \quad (2.10)$$

Since we have chosen l^* such that $t(l^*) = -\frac{1}{2}$,

$$e^{l^*} \sim t^{-\nu} . \quad (2.11)$$

Combining Eqs. (2.10) and (2.11) yields Eq. (2.5) with $\theta = \frac{1}{2}$.

III. DISCUSSION

The result of our calculations is that the exponents (2.7) governing the widths of the commensurate phases are modified, and generally increased, compared with the mean-field exponents (1.3). For instance, for $k=3$ mean-field theory gives $\Delta_3 \sim t_c$, but the renormalization group gives $\Delta_3 \sim t_c^{\xi_3}$. Extrapolating Eq. (2.7) to $\epsilon = 1$ $(d=3)$ yields $\xi_3 \simeq 1.2$. Padé approximants yield $\xi_3 \sim 1.2-1.4$, so the cusp becomes sharper. All Padés give higher values than mean-field theory, so we conjecture that the shape becomes sharper also for $k > 3$. For large k we have

$$\xi_k \sim \frac{k}{2} f(k\epsilon), \quad f(x) \sim 1 + \frac{x}{5} - \frac{2}{25}x^2 .$$

Figure 1 shows schematically the behavior near T_c. Since the widths decrease to zero as t^{ξ_k}, the commensurate phases will not overlap when t is small enough, and they do not fill out the phase diagram (see the discussion by Pokrovsky, Ref. 14). We thus have an infinity of commensurate phases, i.e., the "devil's staircase" survives fluctuations in the limit $T \rightarrow T_c$.

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