PHYSICAL REVIEW B VOLUME 22, NUMBER 11 1 DECEMBER 1980

Critical behavior of commensurate-incommensurate phase transitions in two dimensions

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(Received 7 May 1980)

It is shown that there are no critical divergences on the commensurate side of the commensurate-incommensurate transition in the two-dimensional sine-Gordon system, whereas on the incommensurate side there are divergences of the specific heat and of the correlation length. The critical exponents are determined. The results are explained in terms of fluctuating domain walls between commensurate regions. This allows a generalization of some of the results to more complex systems.

In a two-dimensional system a long-range ordered (LRO) phase with a continuous symmetry is not possible at finite temperature due to the divergent fluctuations of the Goldstone mode.[1] On the other hand, if the symmetry is discrete there is no Goldstone mode and therefore LRO is possible at $T \neq 0$, the best known example being the two-dimensional Ising model.[2] A crossover between these two situations is realized by the transition from the commensurate (C, discrete symmetry) to the incommensurate (IC, continuous symmetry) state. The observation of such a transition in gas monolayers adsorbed on solid surfaces[3–6] has lead to considerable theoretical interest in the problem.[7–10]

Here we investigate the critical behavior of the C-IC transition using a simple model free energy functional

$$F = \int dx\,dy \left[\frac{\mu}{2}\left(\frac{\partial u}{\partial x} - \delta\right)^2 + \frac{\nu}{2}\left(\frac{\partial u}{\partial y}\right)^2 + \lambda \cos nu \right] \quad , \quad (1)$$

where u is an atomic displacement field. The cosine potential favors the commensurate state, whereas a finite δ favors the incommensurate state. The zero-temperature properties[11] and the phase diagram[9] of this model have been intensively investigated: For $|\delta|$ smaller than some critical value δ_c the C phase is stable. This state is invariant under the discrete symmetry operation $u \rightarrow u + 2\pi/n$ and is therefore stable at $T \neq 0$.[9] On the other hand, for $|\delta| > \delta_c$ an IC phase is realized, consisting of large commensurate domains separated by walls parallel to the y direction. The energy of this state is invariant under an infinitesimal translation of the walls, i.e., there is a continuous symmetry and no LRO can exist at $T \neq 0$. We treat the statistical mechanics of Eq. (1) using the equivalence to the ground-state properties of a one-dimensional quantum Hamiltonian[12] which in our case reads

$$H_1 = \frac{c}{2\rho} \int \left[\pi^2(x) + \left(\frac{\partial \phi}{\partial x}\right)^2 + v \cos\frac{n}{\sqrt{c}}\phi - \gamma \frac{\partial \phi}{\partial x} \right] dx \quad , \quad (2)$$

with $c^2 = \mu\nu/T^2$, $\rho = \nu/T^2$, $v = 2\sqrt{\nu/\mu}\,\lambda/T$, and $\gamma = 2\delta\sqrt{c}$. ϕ and π are a Bose field and its conjugate momentum density, respectively. H_1 is the quantum sine-Gordon system with an additional gradient term arising from the δ term in Eq. (1). For $\gamma = 0$ there is an instability at $n^2/c = 8\pi$.[13] This corresponds to the disordered-commensurate transition at $\delta = 0$ and $T = T_0$.[10] We do not consider this special point but look rather at the C-IC transition for $\delta \neq 0$, $T < T_0$, so that $n^2/c < 8\pi$. H_1 may be transformed into a one-dimensional interacting spinless fermion model[14] using the boson representation of single fermion operators.[15] From this representation it follows that the gradient term in H_1 is equivalent to a chemical potential for the fermions. The fermion Hamiltonian equivalent to H_1 may then be written as

$$H_2 = \frac{1}{2\rho} \left[\sum_k [(c'k + \mu_0) a_k^\dagger a_k - (c'k - \mu_0) b_k^\dagger b_k + \Delta_0/2 (a_k^\dagger b_k + b_k^\dagger a_k)] + \frac{2\pi c}{L} \sinh 2\varphi \left(2 \sum_p \rho_1(p)\rho_2(-p) - f_1 \sum_p [\rho_1(p)\rho_1(-p) + \rho_2(-p)\rho_2(p)] \right) \right] \quad , \quad (3)$$

where a_k and b_k are operators for right- and left-going fermions, ρ_1 and ρ_2 the corresponding density operators, $e^{2\varphi}=4\pi c/n^2$, $c'=2c(\cosh 2\varphi + f_1 \sinh 2\varphi)$, $\mu_0=4\pi\delta c^2/n$, $\Delta_0=2\pi\alpha_0 c v$, and α_0 is a cutoff which may be identified with the lattice constant. As the last sum in Eq. (3) is the kinetic energy represented in terms of density operators[18] it is easy to see that f_1 may be chosen arbitrarily in H_2. We now diagonalize the first line in Eq. (3) by a Bogolyubov transformation and obtain

$$H_2=\frac{1}{2\rho}\left[\sum_{k,n=1,2}(\epsilon_{kn}+\mu_0)c_{kn}^{\dagger}c_{kn}+H_{\rm int}\right] , \quad (4)$$

where $\epsilon_{kn}=(-1)^n(c'^2k^2+\Delta_0^2/4)^{1/2}$ and $H_{\rm int}$ is the interaction term in Eq. (3) expressed in terms of the c_{kn} operators. If there are no particles above the gap $H_{\rm int}$ leads only to a gap renormalization $\Delta_0\to\Delta$.[16] For $\mu_0<-\Delta/2$ the 2-states are filled[17] up to some value k_c and the interaction between the 2-particles has to be treated properly. If one is only interested in the long-distance properties of the system (i.e., $r>k_c^{-1},c/\Delta$) the behavior is completely determined by the 2-particles and the spectrum of these particles may be linearized about the Fermi points $\pm k_c$. Choosing $f_1=1/(1+8c'^2k_c^2/\Delta^2)$ the Hamiltonian for the 2-particles is

$$H_3=\frac{1}{2\rho}\left[\frac{2\pi v_c}{L}\sum_{p>0}[\sigma_1(p)\sigma_1(-p)+\sigma_2(-p)\sigma_2(p)] + \frac{4\pi c}{L}\sinh 2\varphi f(k_c)\sum_p \sigma_1(p)\sigma_2(-p)\right] , \quad (5)$$

with $v_c=c'^2k_c(c'^2k_c^2+\Delta^2/4)^{-1/2}$, $f(k_c)=v_c^2/c'^2$, and $\sigma_{1,2}$ are fermion density operators analogous to the ρ operators in Eq. (3). We note that the ratio of the interaction strength to the Fermi velocity v_c vanishes linearily with k_c, due to the special choice of f_1. Thus the linearization of the single-particle spectrum is well justified. H_3 is a Tomonaga-Luttinger Hamiltonian and is easily diagonalized by a unitary transformation.[18] Here we have only considered the case $\mu_0<-\Delta/2$, so that 2-states are filled. However, the treatment for $\mu_0>\Delta/2$ is completely analogous and requires only the replacement of the 2-particles by holes in the 1-band.

We now use the above results to consider the C-IC transition in our original system [Eq. (1)]. The mean "incommensurability" is

$$I=\frac{1}{L}\left\langle\int\frac{\partial u}{\partial x}dx\right\rangle_F=-\frac{2\pi}{Ln}\sum_{k,n=1,2}\langle c_{kn}^{\dagger}c_{kn}-\tfrac{1}{2}\rangle_{H_2} , \quad (6)$$

where $\langle\cdots\rangle_F$ and $\langle\cdots\rangle_{H_2}$ are the thermodynamic average with the functional F and the ground-state average of H_2, respectively. If $|\mu_0|<\Delta/2$ all 1-states are occupied, all 2-states are empty, so that the system is commensurate. The phase boundary to the IC state is $\delta_c(T)=n\Delta/(8\pi c^2)$. This leads to the known C-IC phase diagram.[9] For small k_c the interaction strength in H_3 vanishes,[19] and we may thus use the single-particle spectrum of Eq. (4) to determine k_c, with the result $k_c=4\pi c^2(\delta^2-\delta_c^2)^{1/2}/(nc')$, and from Eq. (6) we obtain $I\propto \mathrm{sgn}\delta(\delta^2-\delta_c^2)^{1/2}$. The square-root dependence is in agreement with previous results[9,20] obtained at a special temperature so that $\varphi=0$ in our notation. The incommensurability I is equal to the density of domain walls in the system. As a wall changes u by $\pm 2\pi/n$, from Eq. (6) it is natural to interpret the 1-holes and 2-particles as walls associated with a change of u by $2\pi/n$ and $-2\pi/n$, respectively. If δ becomes larger the interactions are no more negligible and no simple expression for k_c can be given. However, for large $|\delta|$ the presence of the gap is unimportant and from Eq. (3) one easily obtains $I=\delta$, as to be expected.

The free energy density of the system [Eq. (1)] is given by the ground-state energy of the equivalent quantum Hamiltonian, so that the specific heat is easily calculated. Inside the C region, i.e., for $|\delta|<\delta_c(T)$, there is only a monotonic variation of the ground-state energy if μ_0 or T is varied, with no singularity for $\delta\to\delta_c(T)$. Therefore *there is no divergence of the specific heat as the C-IC transition is approached from the commensurate side.* Approaching the transition from the IC side the energy of the filled 2-states varies like k_c^3 for $k_c\to 0$. The specific heat upon approaching the transition from the incommensurate side then follows

$$C\propto T_c\delta_c(T_c)(T-T_c)^{-1/2} , \quad (7)$$

i.e., the transition has a critical exponent $\alpha=\frac{1}{2}$. We remark however that at the transition at $\delta=0$, $T=T_0$ this divergence vanishes due to the factor δ_c.

The long-range behavior of the correlation function $K(x,y)=\langle\exp[i(u(x,y)-u(0,0))]\rangle_F$ can be easily calculated as u can be represented in terms of the Bose operators $\sigma_{1,2}$ with the result

$$K(x,y)=e^{iIx}\left[k_c^2\left[x^2+\frac{v'^2T^2}{4\nu^2}y^2\right]\right]^{-\eta} , \quad \eta=\frac{1}{n^2}e^{2\zeta} , \quad (8)$$

with $\tanh 2\zeta=-2c\sinh(2\varphi)f(k_c)/v_c$ and $v'=v_c\,\mathrm{sech}2\zeta$. For large incommensurability one has $\eta=T/(4\pi\sqrt{\mu\nu})$, i.e., K shows the typical nonuniversal behavior of the two-dimensional continuum XY model.[21] Near the transition ($k_c\to 0$) η goes to the universal value n^{-2}

$$\eta=\frac{1}{n^2}\left[1-\frac{4ck_c}{\Delta}\sinh 2\varphi\right] . \quad (9)$$

Before discussing the critical behavior we remark that the treatment given above is based on the smallness of $ck_c \sinh 2\varphi/\Delta$. Sufficiently near to the C-IC transition this is always satisfied except for $T=0$ and $T=T_0(\Delta=0)$. Therefore our results are valid inside the whole temperature interval $0<T<T_0$.

We now discuss our results. For large δ the system cannot fit into the cosine potential, thus leading to the free-field behavior of the continuum XY model. With decreasing δ the system gains energy by forming commensurate regions separated by walls. At $T=0$ the elementary excitations of this state are acoustic phonons, representing oscillations of the wall positions, which are separated by a gap at $q=k_c$ from the oscillation modes of the commensurate regions.[22] As the 2-particles in H_2 represent the walls the spectrum of H_3 gives the elementary excitation spectrum of the walls leading to a longitudinal sound velocity vanishing linearly with k_c. Minimizing the free energy calculated with this sound velocity with respect to k_c leads immediately to $k_c \propto (\delta-\delta_c)^{1/2}$ and $\alpha=\frac{1}{2}$. This shows that the critical behavior is due to the harmonically interacting walls.

The correlation function K shows an interesting crossover from the nonuniversal behavior of the XY model to a universal exponent n^{-2} near the transition. In that region K becomes very anisotropic, reflecting the fact that the walls have a finite line tension acting against the deformation of a single wall, whereas the interwall force vanishes for $k_c \rightarrow 0$. Therefore the length scale of fluctuations is k_c^{-1} in the x direction, but proportional to k_c^{-2} in the y direction, leading to different critical exponents $\nu_x=\frac{1}{2}$ and $\nu_y=1$. Their mean value $\bar{\nu}=\frac{3}{4}$ fulfills the scaling law $\bar{\nu}=1-\alpha/2$.

The absence of critical divergences in the commensurate state may easily be understood noting that the creation of a wall crossing the whole system requires an infinite energy. Therefore the only thermodynamical fluctuations of the C phase are *closed* loops of walls [Fig. 1(a)]. It is easy to see that $\partial u/\partial x$ integrated over such a configuration vanishes, or, physically, equal parts of the total wall length win and lose energy by the incommensurability energy. As the energy of the fluctuations is independent of δ there are no critical fluctuations for $\delta \rightarrow \delta_c(T)$. The same argument applies to a system with square symmetry,

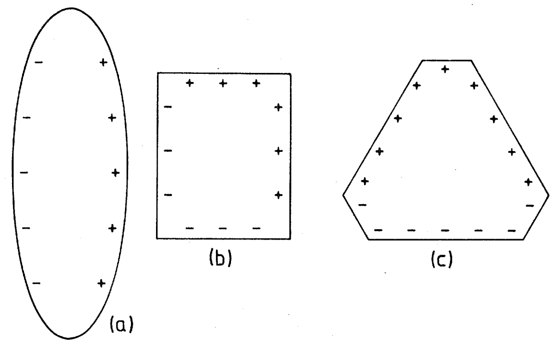

FIG. 1. Fluctuating wall configurations in the C phase of a system with (a) uniaxial [Eq. (1)], (b) rectangular, and (c) hexagonal symmetry. Plus and minus signs denote parts of the walls gaining or losing energy due to the incommensurability term, respectively.

where there are walls parallel to the y and to the x direction [Fig. 1(b)]. On the other hand, for hexagonal symmetry three different directions of walls are allowed and therefore configurations like Fig. 1(c) give rise to critical fluctuations in the C region.

Up to now two-dimensional C-IC transitions have been mainly observed in systems with hexagonal symmetry,[3-6] so that one would expect our theory not to apply. However, Bak *et al.*[7] have shown (for $T=0$) that a second-order transition should occur in these systems only if near the transition the system is uniaxial, i.e., if there are only walls along one direction. In this case there should therefore be the asymmetric (and anisotropic) critical behavior of the model treated here. It would be interesting to observe this experimentally. However, the region of uniaxial modulation may be very narrow so that the interaction of the walls with the periodic substrate (the Peierls force) and impurity effects, neglected here, may become important. Another interesting point is the absence of critical behavior on the C side of the transition in systems with rectangular (or rhombic) symmetry. This should be observable in a system of suitable symmetry.

The author would like to thank J. Friedel, S. Doniach, P. Lederer, and T. Garel for helpful conversations.

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