PHYSICAL REVIEW B VOLUME 28, NUMBER 11 1 DECEMBER 1983

Commensurate-incommensurate transitions and a floating devil's staircase

B. Horovitz,* T. Bohr,† J. M. Kosterlitz‡ and H. J. Schulz§
Einstein Center for Theoretical Physics, The Weizmann Institute of Science, Rehovot, Israel
(Received 6 September 1983; revised manuscript received 24 October 1983)

Renormalization-group equations for the uniaxial commensurate-incommensurate (C-IC) transition in two dimensions are derived. The soliton density ρ is a nonanalytic function of the misfit parameter μ even at high temperatures where only a floating phase (i.e., algebraic correlations with exponent η) is possible. The singularity at $\mu \to 0$ is $\rho - T\mu \sim \mu^{\eta-3}$, where T is temperature. In the (T,μ) plane the floating phase is singular therefore on all lines where its density (relative to the substrate) is rational; this is the remnant of the low-temperature devil's staircase. At low temperatures a matching procedure with the fermion approach is obtained.

Monolayers adsorbed on substrates of uniaxial symmetry exhibit a variety of phase transitions. Commensurate (C)-incommensurate (IC) transitions were found in Xe/Cu(110) (Ref. 1) and H/Fe(110) (Ref. 2), C-fluid transitions in H/Fe(110) (Ref. 2) and Ba/Mo(112) (Ref. 3), and IC-fluid transition in Pb/Cu(110) (Ref. 4). The theory of the uniaxial C-IC phase transition has largely been based on the sine-Gordon model using fermion-boson transformations[5-9] or Bethe-ansatz techniques.[10,11] Within the continuum formulations[5-9,11] the region $\beta^2 > 8\pi$ is inaccessible, but precisely there renormalization-group (RG) treatment is possible. In Ref. 11 the RG equations for the pure X-Y model (i.e., the system with no domain walls) were applied to complement the Bethe-ansatz solution. In order to implement these equations in a system with walls it was postulated that renormalizations should stop at a length scale comparable with the distance between walls, since the system behaves on larger length scales as incommensurate.

In the present paper we actually derive the RG equations valid in a system with a finite density of walls. Since there has been a considerable confusion as to the nature of these equations and their interpretation, we shall carefully state the boundary conditions used and our cutoff procedure.

If T_0 is the maximal temperature for the commensurate phase, we find that for $T < T_0$ the RG equations flow to the regime where the fermion description is valid. We then recover the result[10,11] that the C-IC phase boundary near T_0 is $\mu \sim \exp-(T_0-T)^{-1/2}$, where μ is the chemical potential. When $T > T_0$ the RG equations indeed show that the temperature renormalization effectively stops at the length scale given by the wall spacing. In this case the system is commensurate only when $\mu = 0$; it is a floating phase (i.e., algebraic correlations) for all μ. Yet we find a singularity in the free energy as $\mu \to 0$. It corresponds to a third-order transition when T is near T_0, and changes to higher-order transitions successively as temperature is increased. In terms of the correlation exponent $\eta_0 = \eta(T, \mu=0)$ the singular term is $\sim \mu^{\eta_0-2}$. At $T = T_0$ ($\eta_0 = 4$) the singularity is $\mu^2/\ln\mu$. A similar singularity appears in η itself in agreement with Ref. 11; i.e., $\eta - \eta_0 \sim -\mu^{\eta_0-4}$ and $\eta - 4 \sim -\ln^{-1}\mu$ at T_0.

At low temperatures the adsorbant can form various commensurate phases of periodicity p/q relative to the substrate periodicity, where $p \geq q$ are reduced integers. The sequence of phase transitions at all rational p/q corresponds to a devil's staircase.[12] For $p \geq 5$ dislocations are irrelevant near the C-IC transition and a floating phase separates the C and fluid phases.[13] Our results then show that even within this floating phase there are singularities on all rationals with $p \geq 5$. The staircase is now worn out by fluctuations; each step is a singularity in some derivative of $\rho(\mu)$. For larger p the C phase appears at lower temperature;[12] thus the singularity is weaker for larger p when μ varies at a constant temperature within the floating phase. We call this path of singularities in derivatives a "floating" devil's staircase.

Consider the two-dimensional sine-Gordon with a chemical potential μ which couples to the soliton density $\rho = \int dx_1\, \partial\psi/\partial x_1/(2\pi \int dx_1)$; each turn of the field $\psi(x_1,x_2)$ by 2π in the x_1 direction is a soliton wall extending through the x_2 direction. The Hamiltonian (or action) is

$$\tilde{A}\{\psi\} = \int d^2x \left[\frac{1}{8\pi^2 T} (\vec{\nabla}\psi)^2 - \frac{y}{a^2}\cos\psi - \mu\rho \right] , \qquad (1)$$

where T is proportional to the temperature, y is the substrate pinning potential, and a is the lattice constant. A direct RG treatment of Eq. (1) as previously attempted[14] is not justified. The reason is that μ induces singular terms in the field ψ of the form ρx_1. These terms cannot be Fourier expanded and an RG integration of ψ itself is not straightforward. Instead we define a field $\phi(x_1,x_2)$ with periodic boundary conditions such that

$$\psi(x_1,x_2) = \phi(x_1,x_2) + 2\pi\rho x_1 \ . \qquad (2)$$

Equation (1) corresponds to a Grand canonical ensemble where the soliton density ρ is integrated. Instead we use a canonical ensemble with a fixed ρ with the action

$$A\{\phi\} = \int d^2x \left\{ \frac{1}{8\pi^2 T} \left[\left(\frac{\partial\phi}{\partial x_2}\right)^2 + (1-\zeta)\left(\frac{\partial\phi}{\partial x_1}\right)^2 \right] - \frac{y}{a^2}\cos(\phi + 2\pi\rho x_1) \right\} , \qquad (3)$$

where ζ represents anisotropy. (The free energy has an additional $\rho^2/2T$ term.) An RG integration on ϕ is now possible; formally it is similar to that of Eq. (1) except that ρ is a *fixed* boundary condition and is not allowed to be renormalized.

We proceed to derive RG equations by integrating the high-momentum components of ϕ.[15-18] A detailed derivation is presented in Kogut's review.[17] The only change is that here the second-order term in y generates anisotropic gradient terms involving averages of $\cos(2\pi\rho x_1)$. The resulting RG equations to second order in y are

$$dy = y\left(2 - \frac{\pi T}{\sqrt{1-\zeta}}\right)\frac{da}{a} \quad , \tag{4a}$$

$$dT = -y^2T^3f_1(\rho a)\frac{da}{a} \quad , \tag{4b}$$

$$d\zeta = -\zeta y^2T^2f_1(\rho a)\frac{da}{a} + y^2T^2f_2(\rho a)\frac{da}{a} \quad . \tag{4c}$$

The free-energy change after the RG integration is

$$dF = -\frac{\zeta}{8\pi}\frac{da}{a^3} - y^2Tf_3(\rho a)\frac{da}{a^3} \tag{5}$$

and the functions $f_n(\rho a)$ $(n = 1, 2, 3)$ are

$$f_1(\rho a) = \frac{2\pi^3}{\rho a}\int_0^\infty d\xi\, \xi^3K_1(\xi)J_1(2\pi\rho a\xi)$$
$$= 32\pi^4[1 + (2\pi\rho a)^2]^{-3} \quad , \tag{6a}$$

$$f_2(\rho a) = 2\pi^4\int_0^\infty d\xi \xi^4K_1(\xi)J_2(2\pi\rho a\xi)$$
$$= 96\pi^4(2\pi\rho a)^2[1 + (2\pi\rho a)^2]^{-4} \quad , \tag{6b}$$

$$f_3(\rho a) = \pi^2\int_0^\infty d\xi\, \xi^2K_1(\xi)J_0(2\pi\rho a\xi)$$
$$= 2\pi^2[1 + (2\pi\rho a)^2]^{-2} \quad , \tag{6c}$$

where K_1 and J_n are Bessel functions. A procedure with a sharp momentum cutoff leads to $J_0(\xi)$ instead of $\xi K_1(\xi)$ in the integrals above. The sharp cutoff procedure leads to diverging integrals.[17] Using a smooth cutoff where a mass term represents the cutoff[16,18] leads to Eqs. (6a)–(6c). Our results below are insensitive to these cutoff-dependent details.

Equation (3) is equivalent to a Coulomb gas in an imaginary field ρ. The RG equations for this problem show[19] that ρ is renormalized. (Similar equations are given in Ref. 14.) In our approach ρ is fixed and instead ζ is renormalized. Note also that the Bessel functions J_n are averaged in Eqs. (6a)–(6c) and the oscillations that lead to multiple fixed points[14] disappear.

For $\rho = 0$ the anistropy ζ [Eq. (4c)] is an irrelevant variable and the RG equations reduce to those of the x-y model.[20] For $\rho \neq 0$ an anisotropy is generated; starting from $\zeta = 0$ the generated ζ is of order y^2. To lowest order in y we therefore have $\zeta = 0$ in Eq. (4a) and only the y and T equations are coupled.

For $\rho = 0$ a phase transition at $T_0 = 2/\pi + [8f_1(0)/\pi^5]^{1/2}y$ $(y \ll 1)$ separates the region where y is relevant $(T < T_0)$ or irrelevant $(T > T_0)$ (see Fig. 1). When y is relevant and $\rho \neq 0$ the system has two length scales—the correlation length ξ of the $\rho = 0$ case,[20] $\xi \sim \exp(T_0 - T)^{-1/2}$, and the mean distance between solitons $1/\rho$. If $\xi < \rho^{-1}$ increasing the lattice constant up to ξ is insensitive to ρ [$f_1(\rho a)$ is essentially constant for $\rho a \ll 1$]. The RG equations then increase y to order 1 and T is now below $2/\pi$ (curve C in Fig. 1); in this regime the fermion approach[5-9] is valid. In fact the fermion procedure is suspect when $T \to T_0$. The combination with the RG resolves this difficulty—the length scale of the fermions is identified as the correlation length ξ of the commensurate $(\rho = 0)$ phase. The soliton energy is then $E_s \sim \xi^{-1}$ (Refs. 5 and 7–9) and since the C-IC phase boundary of Eq. (1) is $E_s = \mu_c$ we obtain

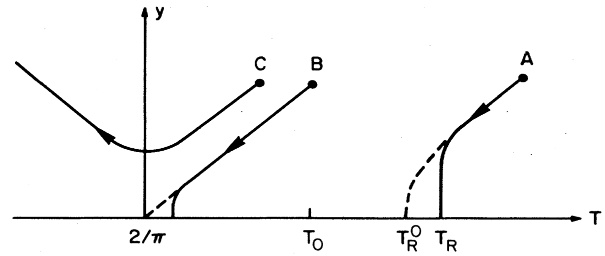

FIG. 1. RG trajectories for finite soliton density $\rho \neq 0$ (solid lines) and for $\rho = 0$ (start at A,B,C and continue into dashed lines when present). The starting points are all on a line $y =$ const (~ substrate potential) and T_0 is the C-IC transition temperature (point B) for that value of y. For $T \geq T_0$ (cases A,B) T stops renormalizing when $\rho a \gtrsim 1$. For $T < T_0$ and $\rho\xi < 1$ (case C) trajectory flows into regime where fermion description is valid.

$$\mu_c \sim \exp - (T_0 - T)^{-1/2} \quad . \tag{7}$$

Sufficiently near this line $\rho(\mu)$ is small so that $\xi < \rho^{-1}$ and the fermion result[5-9] $\rho \sim (\mu - \mu_c)^{1/2}$ is valid.

Integrating the RG equations to the region $\rho a \gtrsim 1$ should show that y is irrelevant since for $\rho \neq 0$ the system is always IC. The anisotropy ζ indeed tends to make y less relevant in Eq. (4a). From the fermion approach[7] we know that the system becomes extremely anisotropic with $1 - \zeta \sim (\rho\xi)^2$ as $\rho\xi \to 0$. The RG equation cannot reproduce this since in the region $\xi < a < \rho^{-1}$ higher-order terms in y are required.

Consider next the high-temperature region $T > T_0$. In this case y is irrelevant and the only length scale is ρ^{-1}. For $\rho = 0$ the T,y trajectory is a hyperbola[20] which intersects the $y = 0$ axis at a renormalized temperature T_R^0 (Fig. 1), where

$$(2 - \pi T)^2 - (2 - \pi T_0)^2 = (2 - \pi T_R^0)^2 \quad . \tag{8}$$

The correlation function $\langle \exp[i\phi(x) - i\phi(0)]\rangle \sim r^{-\eta}$ can also be used to identify T_R^0; when $y = 0$ the system is Gaussian with $\eta_0 = 2\pi T_R^0$, where $\eta_0 = \eta$ $(T, \mu = 0)$. From Eq. (4a) the asymptotic form of y^2 as $a \to \infty$ is

$$y^2 \sim a^{4 - 2\pi T_R^0} = a^{4-\eta_0} \quad . \tag{9}$$

When $\rho a \ll 1$ the RG flow satisfies Eq. (9) for $a < \rho^{-1}$. For $a > \rho^{-1}$ the functions $f_n(\rho a)$ [Eqs. (6a)–(6c)] decrease rapidly and the pinning potential ($\sim y$) stops contributing to the free energy [Eq. (5)]. The reason is that when $a > \rho^{-1}$, $\phi(x_1,x_2)$ must vary more slowly than $2\pi\rho x_1$ and then $\cos(\phi + 2\pi\rho x_1)$ in Eq. (3) averages to zero.

The free energy (5) can now be evaluated. The function $f_3(\rho a)$ induces a cutoff at $a \sim \rho^{-1}$ with a free-energy term

$$-\int^{\rho^{-1}} a^{1-\eta_0}da \sim \rho^{\eta_0 - 2} \quad .$$

Equivalently, the integration can be carried to ∞ with $f_3(\rho a)$ retained. The anisotropy term in (5) leads to a similar term so that the final free-energy density has the form (for $\rho \to 0$)

$$F = \frac{\rho^2}{2T} + C_1\rho^{\eta_0 - 2} \quad , \tag{10}$$

where C_n $(n=1,2,\ldots)$ here and below are constants independent of ρ; $C_n>0$ and are of order y^2. In terms of the chemical potential $\mu=\partial F/\partial\rho$ we obtain (for $\mu\to 0$)

$$\rho=T\mu-C_2\mu^{\eta_0-3} \quad . \tag{11}$$

At the transition $T=T_0$ ($\eta_0=4$) we have $y\sim\ln^{-1}(a/a_0)$, where a_0 is the initial lattice constant. The leading singularity then contributes

$$F=\frac{\rho^2}{2T}-C_3\frac{\rho^2}{\ln(\rho a)} \quad , \tag{12}$$

and therefore

$$\rho=T\mu+C_4\mu/\ln\mu \quad . \tag{13}$$

The C-IC transition in a (discrete) sine-Gordon model can be transformed into a six-vertex (6V) model in both a horizontal and a vertical field,[10] which is exactly solvable. The fields correspond to the chemical potential μ in Eq. (1), the polarization of the 6V model is equivalent to the soliton density ρ, and $T>T_0$ ($T<T_0$) corresponds to $\Delta>-1$ ($\Delta<-1$) in the 6V model (for the definition of Δ and a general discussion of the 6V model see Lieb and Wu[21]). Following an analogous calculation for the *XXZ* spin chain,[22] one finds for $\Delta>-1$

$$F(\rho)-F(0)\propto\rho^2+D\rho^{2(\pi+\nu)/(\pi-\nu)} \quad ,$$

with $\Delta=-\cos\nu$, and a rather lengthy expression for the constant D. Now, the analog of $\cos\phi$ in the 6V and *XXZ* models is the umklapp operator[23] O_{40}, so that $\eta_0=2x_{40}$. Further $x_{40}=4/x_{01}$, and x_{01} is the thermal exponent of the eight-vertex model, known from Baxter's solution:[24] $x_{01}=2(1-\nu/\pi)$. Consequently, $\eta_0=4\pi/(\pi-\nu)$, and from Eq. (14)

$$F(\rho)-F(0)\propto\rho^2+D\rho^{\eta_0-2} \quad ,$$

in agreement with our RG result, Eq. (10). Also, for $\Delta=-1$, the logarithmic term in Eq. (12) can be recovered in the 6V model.

These results show that the free energy is nonanalytic *within* the floating phase as $\mu\to 0$. The line $\mu=0$ is a singular line for all $T\geqslant T_0$ up to the transition to the fluid phase. The singularity becomes weaker for higher temperatures since η_0 increases with T. If $[\eta_0]$ is the integer part of η_0, then the singularity of Eq. (9) as $\rho\to 0$ corresponds to a transition of order $[\eta_0]-1$. Just above T_0 it is third order, and in general of mth order in the temperature range ($y<<1$)

$$\tfrac{1}{4}(m+1)<T/T_0<\tfrac{1}{4}(m+2) \quad . \tag{16}$$

To complete the picture we evaluate $\eta=\eta(T,\mu)=2\pi T_R$, where T_R is the renormalized temperature in the presence of solitons. Since $f_1(\rho a)$ approaches zero when a increases beyond ρ^{-1}, temperature stops renormalizing at $\rho a\gtrsim 1$ and the trajectory ends at $y=0$ with $T_R>T_R^0$ (Fig. 1). The difference $T_R-T_R^0$ is found by integrating Eq. (4b) (with $\rho=0$ which defines T_R^0) along the dashed trajectory in Fig. 1:

$$T_R^0-T_R\sim-\int_{\rho^{-1}}^{\infty}a^{3-\eta_0}da\sim-\rho^{\eta_0-4} \quad ,$$

which yields

$$\eta=\eta_0+C_5\mu^{\eta_0-4} \quad . \tag{17}$$

At $T=T_0$ ($\eta_0=4$) this is replaced by

$$\eta=4-C_6/\ln\mu \quad . \tag{18}$$

Our results for η are in agreement with those obtained in Ref. 11.

We conclude that a floating incommensurate phase is not a simple Gaussian system. Although y is an irrelevant variable, integration along its trajectory leads to a singularity in the free energy. Such a singularity appears at all commensurate situations where the ratio of the absorbant/substrate lattice constants is a rational p/q. For higher p values T_0 is lower and the corresponding singularity at a given T [Eq. (17)] is weaker. Thus the (T,μ) plane of an incommensurate phase has an infinite number of singular lines; a trajectory crossing these lines is a "floating" devil's staircase.

ACKNOWLEDGMENTS

We thank R. Pelcovits and B. Nienhuis for helpful discussions. We also thank E. Domany and D. Mukamel for organizing a fruitful summer institute. One of us (J.M.K.) acknowledges partial support of a NSF grant, No. DMR-8305022.

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*Also Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545. Present address: Department of Physics, Ben-Gurion University, Beer-Sheva, Israel.

†Also at Orsted Institute, DK-2100 Copenhagen, Denmark. Present address: Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY 14853.

‡Present address: Department of Physics, Brown University, Providence, RI 02912.

§Present address: Institut Laue-Langevin, Boîte Postal 156X, F-38042 Grenoble, France.

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