Incommensurate and commensurate phases in asymmetric clock models

S. Ostlund
Laboratory of Atomic and Solid State Physics, Clark Hall, Cornell University, Ithaca, New York 14853
(Received 15 December 1980)

When the ordinary nearest-neighbor p-state clock model (discrete xy model) is generalized to include asymmetric interactions, an incommensurate phase appears for integer $p \geq 3$ in addition to the usual liquid and commensurate phases. Aside from being theoretically interesting, it is of practical importance in studies of the commensurate-incommensurate transition where the existence of a discrete nearest-neighbor model with this property gives a computational advantage over further-neighbor and continuum models. For $p=3$, the incommensurate phase always has a high degree of discommensuration and a Lifshitz point will occur where the incommensurate, liquid, and commensurate phases coincide. For $p=2$ no incommensurate phase occurs. The system is analyzed at low temperature using a transfer matrix technique recently used by J. Villain and P. Bak to analyze a similar model with further-neighbor interactions.

I. INTRODUCTION

Of particular current interest in statistical mechanics is the investigation of the commensurate-incommensurate (C-IC) transition.[1-5] This transition occurs when a commensurate (C) phase with long-range order melts to an incommensurate or "floating" phase. The commensurate phase has a periodicity which is a rational multiple of the periodicity of the underlying lattice. In two dimensions, the IC phase has algebraic decay of order-parameter correlations and a wave vector describing the order parameter which varies continuously with the temperature and interaction parameters. In the present work, it is found that the nearest-neighbor p-state clock model probably[6,7] has an incommensurate phase when it is generalized to include asymmetric interactions. An interesting result of this analysis is that the three-state asymmetric model has an IC phase while the corresponding symmetric three-state (Potts) model does not. Although results which are similar to those found here have been recently derived for a related model with *second*-neighbor interactions as well as first-neighbor interactions,[1] the results presented here are interesting because the present model may be the simplest model in which an IC phase occurs. The conclusions also imply that the three-state Potts model with ferromagnetic interactions along one axis and antiferromagnetic interactions along the perpendicular axis has a low-temperature phase with algebraic order.

The Hamiltonian of the asymmetric p-state clock model is given by

$$\frac{H}{k_B T} = -\frac{1}{T} \sum_{\langle ij \rangle} \cos\left[2\pi \frac{(n_i - n_j - \vec{R}_{ij} \cdot \vec{\Delta})}{p} \right] , \quad (1.1)$$

where p is integer and the integers n_i and n_j range between 0 and $p-1$. The summation is over the nearest-neighbor sites "i" and "j" of a square lattice and $\vec{R}_{ij}$ is the unit vector between sites i and j

$$\vec{R}_{ij} = (\vec{R}_i - \vec{R}_j)/|\vec{R}_i - \vec{R}_j| , \quad (1.2)$$

and $\vec{\Delta} = \Delta \hat{x}$. Each bond is counted once. For $\Delta = 0$, the model reduces to the ordinary clock model. The parameter Δ causes a tendency for the phase angle $2\pi n_i/p$ to have a continuous rotation as a function of position along the x direction. This competes with the restriction that the phase angle must be discrete and this competition causes the appearance of the C-IC transition.

Note the following symmetries of the partition function $Z(\Delta, T)$

$$Z(\Delta, T) = Z(-\Delta, T) = Z(\Delta + m, T) , \quad (1.3)$$

when m is an integer. This symmetry is easily seen by relabeling the integer variables n_i to $n_{i'}$ at each site along each row parallel to the y axis,

$$n_{i'} = n_i - mx . \quad (1.4)$$

The commensurate phases which occur can be labeled by the average integer progression as one moves parallel to the y axis. The pitch of the phase is defined to be the average value of $n(x,y) - n(x-l,y)$, i.e., the pitch-1 phase has the sequence 0123450123 . . . for the six-state model, while the pitch-2 phase has the sequence 024024 or 135135. Since the symmetry in Eq. (1.3) is valid, it is sufficient to study only the phase diagram for $0 \leq \Delta \leq 0.5$. A consequence of the analysis is that only integral-pitch phases with long-range order exist so that the only ordered phase which needs to be

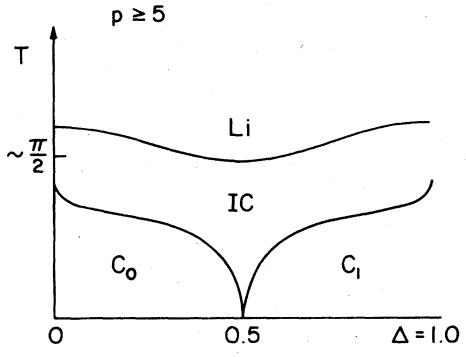

FIG. 1. Phase diagram for the asymmetric $p \geq 5$-state clock model is shown. In an incommensurate (IC) phase, a continuously varying wave vector describes the order. The ferromagnetic pitch 0 and 1 (C_0 and C_1) phase has true long-range order, while the liquid phase has exponential decay of orientational order.

considered explicitly is the pitch zero and possible coexistence with pitch-1 phase. The phase diagram as a function of Δ and T for the various integer values of p, based on the calculation in the present paper is shown in Figs. 1–4. For $p=4$, the commensurate phase melts to a disordered liquid directly only at $\Delta=0$. Otherwise the melting proceeds via an IC floating phase. For $p \geq 5$, the commensurate phase never extends into the liquid.

The Hamiltonian for $p=2$ is equivalent to an Ising model in zero field, and the phase transition between solid and liquid occurs on the self-dual line of anisotropic Ising model[8]:

$$\cos(\Delta\pi) = -\tfrac{1}{2}\, T \ln[\tanh(1/T)] \tag{1.5}$$

for $\Delta \leq 0.5$. There is no floating phase in this case.

For $p=3$, the commensurate phase extends into the liquid but an incommensurate floating phase ex-

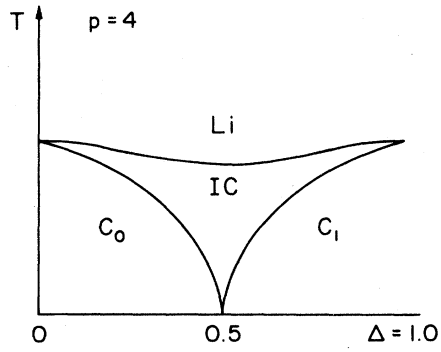

FIG. 2. Transition between solid and liquid occurs only at integer Δ for the four-state asymmetric model. For nonintegral Δ the transition from solid to liquid occurs via the incommensurate phase.

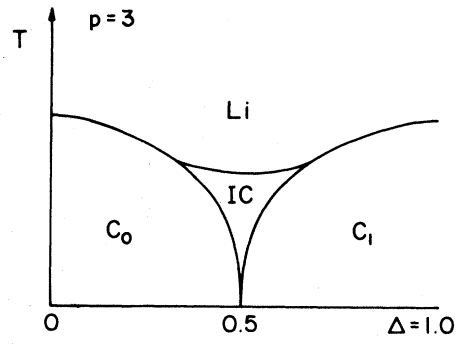

FIG. 3. For $p=3$, the ferromagnetic phase extends into the liquid, while the floating phase occurs for values of Δ near $\frac{1}{2}$ and at low temperature.

ists for values of $\Delta \simeq \frac{1}{2}$. It is found that the average pitch of the floating phase is $\frac{1}{2}$ at $\Delta=\frac{1}{2}$, so that the favored integer sequence is 001122001122 . . . . The line determined by $\Delta=0.5$ is thermodynamically equivalent to the line $\Delta=1.5$ in the three-state model. The latter case corresponds to a three-state Potts model[9] with ferromagnetic interactions along the y axis but antiferromagnetic interactions along x

$$\frac{H}{k_B T} = \frac{1}{T}\sum_{\langle ij\rangle_x} \delta_{n_i,n_j} - \frac{1}{T}\sum_{\langle ij\rangle_y} \delta_{n_i,n_j} \ . \tag{1.6}$$

Thus this model too is expected to have a low-temperature phase with algebraic order. It is interesting to note that this mixed ferro-antiferromagnetic model has a favored integer sequence given by 010101, 020202, or 1212121, obtained from the pitch-$\frac{1}{2}$ sequence via the transformation in Eq. (1.4). The results derived here indicate that this version of the three-state Potts model has algebraic order in the spin order parameter

$$\psi(\vec{R}) = (-1)^x e^{2\pi i n(\vec{R})/3} \tag{1.7}$$

and an xy-like transition[10] to a liquid at finite T.

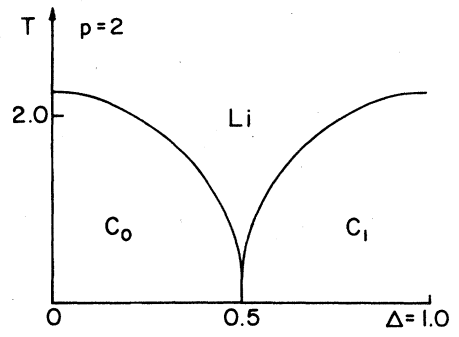

FIG. 4. Case where $p=2$ is equivalent to the Ising model in zero field. No floating phase occurs in this case.

"Locking-in" is believed to occur in three-dimensional (3D) systems, and occurs if there is a phase with long-range order and an arbitrary rational value for the pitch.[5] It should be noted that in none of these models is there a "locked-in" phase at a pitch other than integral values of p.

II. RELATION TO OTHER WORK

The symmetric clock models have been studied in detail by a number of authors.[7] These models have "accidentally commensurate" floating phases,[11] where the reciprocal-lattice vector describing the order parameter is zero. For $p \geq 5$, the incommensurate phase is an extension of these floating phases to off the symmetry axis $\Delta = 0$. The symmetric clock models are self-dual, a property not shared by the asymmetric model, since the dual of an asymmetric clock model has complex (number) interactions.[7,9,12]

A continuum version of the asymmetric xy model in which vortices are neglected has been studied by Schulz.[13] The Hamiltonian studied there was given by

$$\frac{H}{k_B T} = \frac{1}{2} \int dx\, dy \left[K_x \left(\frac{\partial \phi}{\partial x} - \delta \right)^2 + K_y \left(\frac{\partial \phi}{\partial y} \right)^2 + h \cos(n\phi) \right] . \tag{2.1}$$

This model is expected to represent the C-IC transition correctly in the absence of vortices and should therefore accurately represent critical behavior along the C-IC line well below the liquid phase for the clock models also.

It is of interest to compare the present model with the ANNNI[14] and ANNNC models studied in Ref. 1. These systems have the Hamiltonian

$$\frac{-H}{k_B T} = \sum_{\langle ij \rangle_{nn_x}} J_1 \cos\left(\frac{2\pi(n_i - n_j)}{p} \right) + \sum_{\langle ij \rangle_{nn_y}} J_0 \cos\left(\frac{2\pi(n_i - n_j)}{p} \right) + \sum_{\langle ij \rangle_{nnn_y}} J_2 \cos\left(\frac{2\pi(n_i - n_j - 1)}{p} \right) , \tag{2.2}$$

where the summations are over nearest neighbors in the first two terms and over the second neighbors along the y direction in the third term. The site "i" is chosen above or to the right of the site "j." For the value $p = 2$, the model reduces to the ANNNI model studied by Selke and Fisher.[14] Note that the competition between the second-neighbor and first-neighbor interactions gives rise to the incommensurate phases. The asymmetric clock model of the present work is strictly nearest neighbor, and the variation of the parameter Δ changes the commensurability.

In spite of these microscopic differences, the analysis of these two models is very similar with respect to domain walls and vortices. The free fermion analysis in Ref. 1 can therefore be applied with very few modifications to the present problem, and the method will not be discussed in any great detail in subsequent sections. A substantial advantage of the present nearest-neighbor clock model over the ANNNC models occurs with other methods of analysis in which the nearest-neighbor property is an advantage, for instant Monte Carlo analyses or finite-size scaling.

The domain-wall theory of incommensurate overlayers was considered in detail by V. Pokrovsky and A. Talapov.[2,15] The algebraic decay of order-parameter correlations was deduced in their work.

III. FREE FERMION ANALYSIS

Let us consider the Hamiltonian (1.1) in the special case $\Delta = 0.5$ and $T = 0$. In this case, there is an infinite ferromagnetic interaction along each bond in the y direction, resulting in each row parallel to the y axis having the same value for the integer "spin" n_i. Assume that the row at x has spin 0. Then the entire next row can have spin 0 or 1 with equal probability. There is therefore a large ground-state entropy which scales like $\Omega^{1/2}$, where Ω is the system size. (Of course, the ground-state entropy per site is zero in the thermodynamic limit.) Using a 1D transfer matrix, one easily shows that

$$\langle \psi_i \psi_j^* \rangle \simeq \left(\tfrac{1}{2} \right)^{|x_i - x_j|} , \tag{3.1}$$

where $\psi_i = \exp[2\pi i (n_i - \frac{1}{2} x_i)/3]$ and x_i is the x coordinate of site i. The system can be characterized by domain walls where the phase angle increases by $2\pi/p$ as one moves from x to $x+1$. A typical domain structure is shown in Fig. 5(a). The distance between domain walls is at least one lattice spacing, and the number of domain walls n_w cannot exceed L_x, the number of sites of the system in the x direction.

At finite temperature we must consider kinks in the walls, an example of which is shown in Fig. 5(b). These have a probability per unit length γ of occurring, relative to no kink, where γ is given by

$$\gamma = \exp[-2/T \sin^2(\pi/p)] . \tag{3.2}$$

The yth row is described by kinks at $x_1, x_2, \ldots, x_{n_w}$.

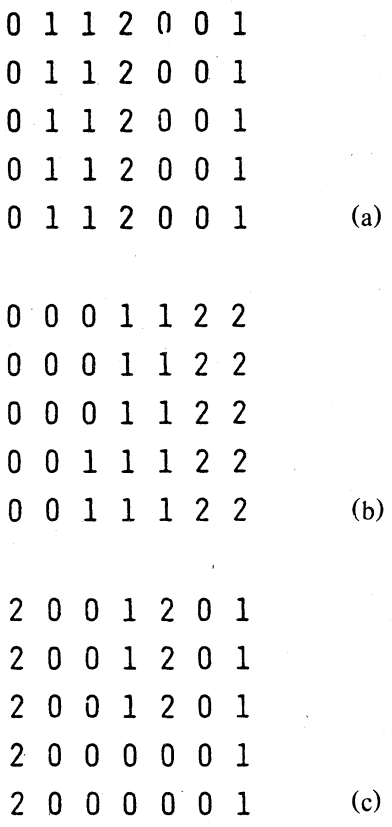

FIG. 5. (a) Typical domain-wall structure for the three-state asymmetric model is shown. The distance between domain walls is two lattice spacings, on the average. (b) A kink in the domain wall between the 0 and 1 domain is shown. This type of excitation destroys long-range order within the rows, and causes the crossover to algebraic order. (c) A vortex consists of three domain walls for $p=3$, which join at a point. This type of excitation causes the floating phase to melt into the fluid.

Thus the "state" of the yth row is written as

$$|y\rangle = |x_1(y), x_2(y) \cdots x_{n_w}(y)\rangle \ . \tag{3.3}$$

The probability that state $|y+1\rangle$ occurs above state $|y\rangle$ relative to the probability that $|y\rangle$ is repeated is given by a transfer matrix $\tilde{T}$ by

$$\langle y+1|\tilde{T}|y\rangle = \gamma^m \ , \tag{3.4}$$

where m is the number of kinks at level y.

A domain wall at (x,y) can be described by a fermion[1] at position x and "time" y. The fermion statistics are essential in keeping the domain walls from crossing, a situation with high energy since a "2" would then appear to the right of a "0", for instance. Thus we can define creation and annihilation operators which obey the usual anticommutation relations and which create or destroy a domain wall at position x

$$|y\rangle = c^\dagger(x_1)c^\dagger(x_2)\cdots c^\dagger(n_w)|\text{vac}\rangle \ , \tag{3.5}$$

where $|\text{vac}\rangle$ is the vacuum state containing no domain walls. In this representation, the transfer matrix can be seen to be approximately given by

$$\tilde{T} = \exp(-H_F) \ , \tag{3.6}$$

where H_F is given by

$$-H_F = \gamma \sum_x c^\dagger(x)c(x-1) + c^\dagger(x-1)c(x) \ . \tag{3.7}$$

This approximate equality is easy to check by expanding the exponential in a power series in H_F.

In the thermodynamic limit, the ground state of H_F dominates the partition function

$$Z_{n_w} = \exp(-L_y\epsilon_0) \ , \tag{3.8}$$

where ϵ_0 is the ground-state energy in the presence of n_w fermions. The ground-state energy is given by

$$-\epsilon_0(n_w) = \frac{2\gamma L_x}{\pi}\sin\left[\frac{\pi n_w}{L_x}\right] \ . \tag{3.9}$$

Therefore the partition function is given by

$$Z_{n_w} = \exp[L_y(2\gamma L_x/\pi)\sin(\pi n_w/L_x)] \ . \tag{3.10}$$

The grand partition function is a sum over n_w of Z_{n_w}

$$Z(\Delta,T) = \sum_{n_w} Z_{n_w} e^{-\mu L_y n_w} \ , \tag{3.11}$$

where $T\mu$ is the chemical potential per unit length of a domain wall

$$\mu = 1/T\{\cos(2\pi\Delta/p) - \cos[2\pi(1-\Delta)/p]\} \ . \tag{3.12}$$

In the thermodynamic limit, the minimum term in Eq. (3.17), occurring at $n_w = \bar{n}_w$, dominates the sum, so that the complete partition function can be evaluated as

$$Z(\Delta,T) = \exp\{L_y L_x[2\gamma/\pi\sin(\pi\rho) - \mu\rho]\} \ , \tag{3.13}$$

where the fermion density ρ is defined to be $\bar{n}_w/L_x$ and satisfies

$$\cos(\pi\rho) = \mu/2\gamma \ . \tag{3.14}$$

Note that the pitch is equivalent to the fermion density.

The phase structure of the original model is therefore apparent. In the range of Δ and T for which the inequality

$$|\mu/2\gamma| \leq 1 \tag{3.15}$$

is valid, the pitch varies continuously with Δ, while for the opposite case, the pitch is either zero or one corresponding to commensurability. The phase boundary is given by the equality of Eq. (3.15), and

Eq. (3.14) determines the pitch as a function of Δ and T. The condition $\mu(\Delta=0)=2\gamma$ provides an estimate for the maximum temperature at which the ferromagnetic phase exists. It remains to show that the order-parameter correlations indeed decay algebraically and that vortices can be neglected. If these conditions are valid, the existence of the floating phase will be considered to be established.

The deviation angle $\phi(x,y)$ is defined by

$$\phi(x,y)=2\pi[n(x,y)-\rho x]/p \tag{3.16}$$

where $n(x,y)$ is the value of the integer clock field at the site (x,y). The order parameter $\psi(\vec{r})$ is defined to be

$$\psi(\vec{r})=e^{i\phi(\vec{r})} \ . \tag{3.17}$$

The correlation function $C(\vec{r})$ defined by

$$C(\vec{r})=\langle\psi(\vec{r})\psi^*(0)\rangle \tag{3.18}$$

can be calculated using the free fermion approximation. Since the algebra of the calculations is very similar to the analogous calculation for the ANNNC model, the details will not be presented here.[1] Indeed, it is found that in the region where the wave vector is continuously varying, that $C(\vec{r})$ decays algebraically

$$C(r)=f(x/y)r^{-\eta} \ , \tag{3.19}$$

where η is given by $\eta=2/p^2$ when vortices are neglected. It is somewhat surprising that η does not depend on temperature. The angular function $f(x/y)$ does depend strongly on both Δ and T.

Since the decay of the angular correlations is algebraic, one can associate the clock model with the xy model at large lengths. Using the Kosterlitz-Thouless (KT) renormalization group,[6] one finds that the (renormalized) exponent η^R is given by

$$\eta^R=\eta+O(y_f) \tag{3.20}$$

when vortices are taken into account.[10] The vortex fugacity is denoted y_f.

A vortex in the present model is shown in Fig. 5(c). Using a simple trigonometric identity one can easily show that the energy of the vortex is p, so that the vortex fugacity is

$$y_f=e^{-p/T} \ . \tag{3.21}$$

The KT analysis also indicates that vortices become unbound when η^R reaches the value $\frac{1}{4}$. The condition for stability of the phase with algebraic order against vortices is therefore given by[1,16,17]

$$\tfrac{1}{4}\geq 2/p^2+\text{const}\ e^{-p/T} \ . \tag{3.22}$$

For sufficiently small temperature, this inequality always holds for $p>2\sqrt{2}$, so that the existence of the floating phase for integer $p\geq 3$ is established. It is satisfying to see that the Ising model is not stable against vortices, in agreement with the known phase diagram for $p=2$. In fact, the equation $\mu=2\gamma$ gives the correct expression for the phase boundary to first order in an expansion in $e^{-2/T}$ of the exact phase boundary given by Eq. (1.5). The calculation of the correlation functions is not applicable to the Ising model however, because the vortices must be taken into account, and these eventually cause the correlations to decay exponentially at large distances.

IV. CRITICAL PROPERTIES

The IC-Li transition is expected to be identical to the ordinary xy transition studied by Kosterlitz and Thouless. There is a correlation length which obeys

$$\xi\propto e^{-t^{-1/2}} \ , \tag{4.1}$$

where $t\propto|T-T_c|$ as the critical line is approached at constant Δ. Only essential singularities proportional to ξ^{-2} occur in the specific heat. The xy "angle field" associated with this transition is given by Eq. (3.16). The exponent η approaches the value $\frac{1}{4}$ with a square-root cusp as the transition line is approached.

The solid-to-liquid transition occurring at $\Delta=0$ is either Ising-like or three-state-Potts-like for $p=2$ or 3. It is consistent with ideas of universality that the transition remains three-state-Potts-like off the symmetry axis until the IC phase is encountered at the Lifshitz point for $p=3$. The properties of this special point cannot be investigated by the present method.

For arbitrary p, the exponent relation $\eta=2/p^2$ is valid close to the entire C-IC line, and this value is also approached at low temperature. Due to the relative divergence of the correlation lengths ξ_x and ξ_y defined below, one must take some care when considering this limit however. For $\Delta\simeq 0$, one must consider closed domain walls, and the present analysis is not expected to remain valid. With these caveats, one can analyze the properties near the IC-C transition by extracting the critical behavior in the free fermion approximation. It can be checked that the results obtained this way indeed agree with the results obtained by Schultz for the Hamiltonian in Eq. (2.1) in the limit of a large field h.

Close to the C-IC transition, the correlation function obeys

$$C(x,y)\propto[(x/\xi_x)^2+(y/\xi_y)^2]^{-\eta/2} \ , \tag{4.2}$$

where the correlation lengths ξ_x and ξ_y obey

$$\xi_x\propto|\Delta-\Delta_c|^{-1/2} \ , \tag{4.3a}$$

$$\xi_y\propto|\Delta-\Delta_c|^{-1} \tag{4.3b}$$

(the y direction lies parallel to the domain walls).

There is therefore a divergence in the anisotropic properties of the correlation function. The pitch ρ obeys

$$\rho \propto |\Delta - \Delta_c|^{1/2} \ . \tag{4.4}$$

There is a specific-heat singularity as the transition is approached from the IC side which scales like ξ_x but the amplitude must vanish as the symmetry point $\Delta = 0$ is approached leaving only the essential singularity characteristic of an xy transition for $p \geq 5$.

The Hamiltonian in Eq. (1.1) is believed to have a Kosterlitz-Thouless transition for $\Delta = 0$ for $p \geq 5$. If, however, the cosine potential is replaced by a potential which is more strongly peaked at $\theta = 0$, there may be a first-order transition directly from the locked phase to the liquid. This situation occurs for the five-state Potts model, which is the limiting case of such a peaked potential. With such a peaked potential, there is then a Lifshitz point possible in the asymmetric model when Δ is not zero and the phase diagram would be represented by Fig. 3 with the IC-Li transition being first order. Since the arguments in Sec. III only depend on the assumption that the energy of a vortex exceeds the energy of a kink, it is expected that any continuous potential replacing the cosine in Eq. (1.1) will result in an IC phase near $\Delta = 0.5$.

V. RELATION TO STRONGLY ADSORBED OVERLAYERS

It has been suggested[12] that the Hamiltonian which is relevant to the melting of a strongly absorbed submonolayer of atoms is given by

$$H = \sum_{\langle ij \rangle} V(\vec{u}_i - \vec{u}_j, \vec{R}_{ij}) + \Delta \sum_{\langle ij \rangle} \vec{R}_{ij} \cdot (\vec{u}_i - \vec{u}_j) \ . \tag{4.5}$$

The vector $\vec{R}_{ij}$ is the lattice vector separating unit cells of the adsorbed solid and $\vec{u}_i$ is the displacement fields which are provided by the substrate in each overlayer unit cell. The term proportional to Δ is a chemical potential term, promoting compression of the overlayer and $V(\vec{u}, \vec{R})$ obeys the symmetry

$$V(\vec{u}, \vec{R}) = V(-\vec{u}, \vec{R}) \ . \tag{4.6}$$

The potential V is periodic in $\vec{u}$, with a periodicity established by the overlayer and the difference vector $u_i - u_j$ is understood to be translated back into the unit cell before the dot product is taken. Thus for a 1×3 overlayer on a square lattice, the displacement field $\vec{u}_i$ takes the values

$$\vec{u}_n = a_0 n \hat{x} \ , \tag{4.7}$$

where a_0 is the lattice constant of the overlayer in the x direction.

The present analysis may be applicable to strongly adsorbed $1 \times p$ overlayers on a square or rectangular lattice. The assumption that the particles not be allowed to occupy interstitial sites is crucial in order to avoid phases with long-range order and an arbitrary rational value of the wave vector describing the order at sufficiently low temperature.[18] With the assumption that only lattice sites are occupied and that only interactions between nearest-neighbor particles are important, one can investigate the phase structure of the resulting model. Admittedly the above assumptions are a very severe limitation on any possible candidate for a system to be mapped into such a model, but the analysis may well turn out to be realistic at least for a certain range of coverage and temperature.

One can approximately calculate the behavior of the structure factor measured in an x-ray experiment. The structure factor is given by

$$S(\vec{q}) = \sum_{\langle nm \rangle} \exp\{i\vec{q} \cdot [\vec{U}(\vec{R}_n) - \vec{U}(\vec{R}_m)]\} \ , \tag{5.1}$$

where the particles are labeled by their location in the commensurate zero-temperature location $\vec{R}_n$ and $\vec{U}(\vec{R}_n)$ is their actual position. This prescription makes sense at low temperature when dislocations are absent. The structure factor can then be evaluated in the free fermion approximation. In this application, the parameter μ is the chemical potential per unit length of a straight domain wall and γ is the fugacity of a kink. These quantities are therefore given by

$$\gamma = \exp[-V_y(a_0/p)/T] \ , \tag{5.2a}$$

$$\mu = V_x(a_0) - V_x[a_0(1 - p^{-1})] + \mu_E \ . \tag{5.2b}$$

The length a_0 is the distance between atoms in the absence of domain walls along the x direction and V_x is the interaction potential along the x axis between adjacent molecules. The parameter V_y is the interaction between molecules separated by a distance a_0/p apart in the x direction and a lattice spacing apart in the y direction. The chemical potential μ_E is the external chemical potential supplied by the gas above the surface.

The vectors $\vec{R}_n$ are defined so that the locations of the atoms at zero temperature in the absence of domain walls are given by integer coordinates. In the presence of domain walls, the location $\vec{U}(\vec{R}_n)$ of this molecule will obey

$$\vec{U}(\vec{R}_m) - \vec{U}(\vec{0}) = \vec{R}_m + [n(\vec{R}_m) - n(\vec{0})]/p\hat{x} \ , \tag{5.3}$$

where $n(\vec{R})$ is the number of domain walls to the left of site $\vec{R}$. Therefore

$$S(\vec{q}) = \frac{1}{\Omega(1+\rho/p)} \times \left\langle \sum_{\vec{R}_m} \exp\left[i\vec{q} \cdot \left(\vec{R}_m + \frac{n(\vec{R}_m) - n(\vec{0})}{p\hat{x}} \right) \right] \right\rangle \ , \tag{5.4}$$

where Ω is the system size in the absence of the domain walls and the extra factor of $(1 + \rho/p)$ is due to the expansion by the walls.

By using the cumulant expansion, one finds that

$$S(\vec{q}) = \sum_{\vec{R}_m} \frac{1}{\Omega(1+\rho/p)} \exp\{i\vec{q}\cdot[\vec{R}_m + \langle n(\vec{R}_m) - n(\vec{0})\rangle/p\hat{x}]\}$$

$$\times \exp\left[-\frac{q_x^2}{2p^2}\langle[n(R_m) - n(0) - \langle n(R_m) - n(0)\rangle]^2\rangle\right] . \quad (5.5)$$

The quantity $\langle n(R_m) - n(0)\rangle$ is nothing but $\vec{R}_m \cdot \hat{x}\rho$ and the expression for the cumulant has been given in Eq. (4.2). One therefore finds that

$$S(q) = \frac{1}{\Omega(1+\rho)} \sum_{\vec{R}_m} \exp[iq_x(1+\rho/p)R_x + iq_y R_y][(R_x/\xi_x)^2 + (R_y/\xi_y)^2]^{-q_x^2/4\pi^2p^2} . \quad (5.6)$$

Near the Bragg condition

$$q_x(1+\rho/p) = 2\pi n_x + \delta_x , \quad (5.7a)$$

$$q_y = 2\pi n_y + \delta_y , \quad (5.7b)$$

where n_x and n_y are integers, one finds that the structure factor has power-law singularities of the form

$$S(q) \propto \frac{1}{(1+\rho)} \xi_x \xi_y \times [(\delta_x\xi_x)^2 + (\delta_y\xi_y)^2]^{[1-n_x^2/(p+\rho)^2]} . \quad (5.8)$$

The critical behavior of ξ_x and ξ_y and ρ is given by Eqs. (4.3)–(4.5). By considering the stability against dislocations (which are equivalent to vortices in this case) one is led to the phase diagram in Fig. 6 for densities less than $\frac{1}{2}$. Away from the C-IC phase boundary, vortices will modify the exponent in Eq. (5.8).

For densities in excess of $\frac{1}{2}$, instead of considering the particles as forming chains, it is appropriate instead to consider holes as forming chains in an otherwise full lattice. The phase structure is therefore qualitatively symmetric in the interchange of particles and hole chains, so that the phase diagram is symmetric in the change of variable

$$n \to 1 - n , \quad (5.9)$$

where n is the particle density relative to the fully packed 1×1 overlayer. Thus the phase diagram for densities near $\frac{5}{6}$ coverage corresponds to the densities near $\frac{1}{6}$ coverage and the holes may form a 1×6 overlayer at sufficiently low temperature.

Let us consider the structure factor in the case where holes form a commensurate $1 \times p$ overlayer lattice and the density is $n = 1 - 1/p$. The structure function $S(q)$ is then given by

$$S(q) = \Omega^2[(1-2/p)\delta_{q,Q_s} + 1/p^2\delta_{q,Q_c}] , \quad (5.10)$$

where Ω is the system area and Q_s are the substrate reciprocal-lattice vectors given by $2\pi(n_x, n_y)$, where n_x and n_y are integers and Q_c are the hole-cell

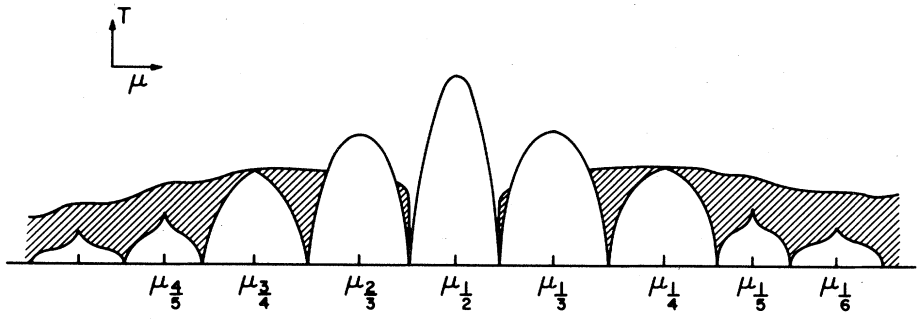

FIG. 6. Phase diagram for an overlayer that orders in chains on a square substrate is shown. The incommensurate floating phases are shown by the shaded parts of the phase diagram. The phase diagram is qualitatively symmetric under the change of variable $n \leftrightarrow 1-n$ where n is density. This reflects the hole-particle approximate symmetry. The chemical potential is plotted along the ordinate, and the chemical potential at $\frac{1}{2}$ coverage is denoted $\mu_{1/2}$. Of course, nonideal effects may invalidate this full phase diagram except over a restricted region of temperature and chemical potential.

reciprocal-lattice vectors $2\pi(n_x/p, n_y)$ where n_i are again integers. There are, therefore, large δ-function peaks in the structure factor at the reciprocal-lattice vectors of the substrate and p weaker δ-function peaks evenly spaced between the substrate peaks due to the hole-hole correlations in the scattering.

In the incommensurate phase the δ-function peaks at Q_c vanish and are replaced by power-law singularities identical in form to the Eq. (5.8).

ACKNOWLEDGMENTS

I wish to thank Julia Yeomans for calling my attention to the manuscripts of J. Villain and P. Bak. Bert Halperin has also been of invaluable assistance in discussions. This work has been supported by the National Science Foundation through the facilities of the Materials Science Center at Cornell University under Grant No. DMR-79-24008.

---

[1]J. Villain and P. Bak (unpublished); J. Villain (unpublished).

[2]For a review of the theory of the commensurate-incommensurate transition, see J. Villain, in *Ordering In Strongly Fluctuating Condensed Matter Systems,* edited by T. Riste (Plenum, New York, 1980), p. 222.

[3]W. Selke and M. E. Fisher, Phys. Rev. B 20, 257 (1979).

[4]M. E. Fisher and W. Selke, Phys. Rev. Lett. 44, 1502 (1980).

[5]P. Bak and J. von Boehm, Phys. Rev. B 21, 5297 (1980).

[6]J. V. Jose, L. P. Kadanoff, S. Kirkpatrick, and D. R. Nelson, Phys. Rev. B 16, 1217 (1977).

[7]See for instance R. Savit, Rev. Mod. Phys. 52, 453 (1980).

[8]H. A. Kramers and G. H. Wannier, Phys. Rev. 40, 252 (1941).

[9]R. B. Potts Proc. Camb. Philos. Soc. 48, 106 (1952); R. J. Baxter, J. Phys. C 6, L5 (1973).

[10]M. Kosterlitz and D. J. Thouless, J. Phys. C 7, 1046 (1974).

[11]D. R. Nelson and B. I. Halperin, Phys. Rev. B 19, 2457 (1979).

[12]S. Ostlund, Phys. Rev. B 23, 2235 (1981).

[13]H. J. Schultz, Phys. Rev. B 22, 5274 (1980). M. den Nijs (unpublished) has also discussed the equivalence of this model with the six-vertex model in an electric field. The six-vertex model is discussed by E. Lieb and F. Wu, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. Green (Academic, New York, 1972), Vol. I. The connection between the 1D free fermion Hamiltonian and the 2D classical vertex models has been studied by F. Y. Wu [Phys. Rev. 168, 539 (1968)].

[14]W. Selke and M. E. Fisher, Z. Phys. B 40, 71 (1980).

[15]V. L. Pokrovsky and A. L. Talapov, Phys. Rev. Lett. 42, 65 (1979).

[16]This inequality was first pointed out to me by Bert Halperin (private communication); see also Refs. 1 and 17.

[17]S. Coppersmith, D. S. Fisher, B. I. Halperin, P. A. Lee, and W. B. Brinkman, Phys. Rev. Lett. 46, 549 (1980); and (unpublished). These authors have also pointed out the connection of the domain-wall theory to adsorbed overlayers and generalize the discussion to triangular overlayer lattices.

[18]S. Aubry, in *Solitons and Condensed Matter Physics,* edited by A. R. Bishop and T. Schneider (Springer, New York, 1978).