QUANTUM MODEL FOR COMMENSURATE-INCOMMENSURATE TRANSITIONS*

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A one-dimensional quantum mechanical model with three states per site is considered. Its ground state shows several commensurate-incommensurate transitions analogous to ones previously studied in two-dimensional statistical mechanics. Using duality arguments, several relations between the phase transition lines can be stated precisely. Further data about the phase diagram can be derived numerically by using strong coupling expansions, including an expansion for the q-dependent mass gap. A fermion analysis is employed to develop exact properties of the incommensurate or floating phase. One new feature is the existence of a Lifshitz point where the critical exponents \( \alpha, \beta \) and \( \gamma \) take the value of the three-state Potts model while the mass gap exponent, \( \nu \), equals one, characteristic of the Ising model.

1. Introduction

In this paper we study phase transitions between commensurate and striped incommensurate phases by means of a one-dimensional quantum hamiltonian. Our model, which has three states per site, is closely related to the chiral three-state clock model introduced by Ostlund [1]. One-dimensional quantum systems are usually related to two-dimensional problems in statistical mechanics via the transfer matrix [2]. Some of the features we observe might therefore be relevant to experimental two-dimensional systems which exhibit striped incommensurate phases, such as xenon monolayers absorbed on copper surfaces [3].

Consider a one-dimensional lattice containing at each site, \( j \), a variable \( \theta_j \) and a conjugate “momentum” variable \( p_j \) which each take on three eigenvalues, 0, 1, 2. These variables do not commute, but obey the commutation relation

\[
e^{ia_p}e^{ia \theta} = e^{ia \theta}e^{ia_p}, \quad a = \frac{\pi}{3}.
\]

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We wish to develop the properties of a model which has the possibility for the 
coexistence of three kinds of phases:

(a) A high temperature or disordered phase in which $e^{i\alpha\theta}$, has a vanishing average 
and short-range correlations.

(b) A low temperature or ordered phase in which $e^{i\alpha\theta}$, has a non-vanishing 
average and a correlation function

$$C_\theta(j-k) = \langle e^{i\alpha(\theta_j - \theta_k)} \rangle$$

(1.2)

which does not die away for large values of the separation, $j-k$. Instead the 
correlation function behaves as

$$C_\theta(j-k) \sim e^{i\alpha Q_\theta(j-k)}.$$  

(1.3)

Here $Q_\theta$ is called the angular pitch of the state. In our ordered or commensurate 
phases $Q_\theta$ takes on integral values. Essentially, the state is ordered so that as $j$ 
increases by one unit $\theta_j$ increases by an amount $Q_\theta$.

(c) Finally, we wish to have an incommensurate or floating phase in which

$$C_\theta(j-k) \sim A(j-k)e^{i\alpha Q_\theta(j-k)},$$

(1.4)

and $Q_\theta$ varies continuously and can thus take on irrational values. This wave vector 
is then incommensurate with the underlying lattice. This phase is distinguished from 
the disordered phase by having the amplitude $A(j-k)$, which is real, decay as a 
power of $j-k$. In the disordered case, we may have a result like (1.4) for large $j-k$ 
but then the amplitude decays exponentially.

One hamiltonian which has the promise of showing this structure is

$$H = -\sum_j \cos(\rho_j - \Delta \rho) a + \beta \cos(\theta_{j+1} - \theta_j - \Delta \theta) a.$$  

(1.5)

Ostlund has analyzed this system for the special case corresponding to $\Delta = 0$. There 
are apparently three phases arranged in the configuration shown in fig. 1. A fermion 
analysis carried out near $\Delta = \frac{1}{2}, \beta = \infty$ shows that in this region $Q_\theta$ varies 
continuously within the floating phase. This phase arises because the kinetic term in $H$ 
allows $\theta_j$ to behave in its long-range correlations as if it were a continuous (gaussian) 
variable instead of an operator with discrete eigenvalues.

In eqs. (1.2)-(1.4) we introduced the pitch $Q_\theta$ by means of the periodicity in the 
long-range behavior of correlation functions. At low temperatures, large $\beta$, it is 
convenient to think of the model in terms of domain walls. The pitch $Q_\theta$ can be 
defined there as the average value of the winding number:

$$Q_\theta \sim \langle \sin(\theta_{j+1} - \theta_j) a \rangle.$$  

(1.6)
The misfit parameter $\Delta_\theta$ favors the presence of clockwise domain walls ($\theta_{i+1} - \theta_i = 1$) when $\Delta_\theta \approx \frac{1}{2}$. These walls are the fermions in the free fermion analysis around $\Delta_\theta = \frac{1}{2}$. The power-law decay of the correlation functions in the incommensurate phase results, in this formulation, from the free meandering of the walls, i.e., the kinetic-hopping-energy of the fermions. In this paper, we consider the special case of the Hamiltonian (1.5) in which $\Delta_\theta = \Delta_\phi$. This situation is especially tractable (and especially interesting) because there is a dual symmetry in which for positive $\beta$ all correlation functions are left invariant under the interchange $\beta \rightarrow \beta^{-1}, p_j \leftrightarrow \theta_{j+1} - \theta_j$. One might then be led to speculate that there are really two pitches, $Q_\theta$ as defined in (1.4), and $Q_p$, defined by

$$C_p(j-k) = \exp \left( ia \sum_{n=k}^{j-1} p_n \right) - A' (j-k) e^{iaQ_p(j-k)}. \quad (1.7)$$

The momentum pitch $Q_p$ governs the periodicity in disorder operator correlation functions, while the angular pitch plays a similar role for the order operators.

Are these two pitches $Q_p$ and $Q_\phi$ really different? What is the interpretation of the momentum pitch $Q_p$ at low temperatures, where $Q_\theta$ has a simple meaning in terms of the density of domain walls?

To examine this question and to find the phase diagram of our model we employ three kinds of analysis. In sect. 2 of this paper a set of exact symmetries are developed, e.g., the duality symmetry just mentioned. Sect. 3 is devoted to the description of a numerical analysis of this model based upon strong coupling series for the free energy, magnetization, and susceptibility and most especially upon series for the mass gap (minimum excitation energy) as a function of wavevector, $q$. Then in sect. 4, we develop a free fermion analysis as a degenerate state perturbation expansion about the points $(\beta = 0, \Delta_\phi = \frac{1}{2}), (\beta = \infty, \Delta_\phi = \frac{1}{2})$ and $(\beta = -\infty, \Delta_\phi = 0)$.

![Fig. 1. Phase diagram for Ostlund's model, $\Delta_\phi = 0$. The dotted line separating the incommensurate (IC) phase from the disordered phase is a line of Kosterlitz-Thouless transitions](image-url)
Based upon the general properties of this perturbation expansion, in sect. 5 we make global statements about our phase diagram.

Before going into detailed analysis, we summarize our results by showing our final, partially derived partially conjectured, phase diagram in fig. 2. (Specific warnings, caveats, etc., about the strength of our conclusions are to be found in the body of the paper.)

The main features of the diagram are:
(a) Critical lines, AB, B'A' in the three-state Potts model universality class, separating disordered phases (with integral values of \( Q_p \)) from ordered phases (which have integral values of \( Q_p \)).
(b) Commensurate-incommensurate (C-I) phase boundaries (dashed) of the type discussed by Pokrovskii and Talapov [4]. Notice that these boundaries equally well separate disordered and incommensurate phases as well as ordered and incommensurate ones.
(c) Two kinds of Lifshitz points (B and B' as well as D and D'). The specific heat, magnetization and susceptibility show three-state Potts behavior at these points; the mass gap goes linearly to zero as in the Ising model.
(d) Several multicritical points C, C', F and F' where fermion expansions may be applied. The behaviour in the neighborhood of these points is, for most purposes, exactly known.
(e) Some points with Kosterlitz-Thouless critical behavior: G, E and E'.

![Phase diagram](image-url)

Fig 2 Phase diagram for the hamiltonian (1.5) with \( \Delta_p = \Delta_p - \Delta \) Data points are obtained from strong coupling series. The vertical scale is distorted for \(|\beta| > 1\).
The ordered and disordered phases can be characterized by integer values of the pitches. In the $\beta \to \infty$, low-temperature limit, the Hamiltonian reduces to

$$H = -\beta \sum_n \cos(\theta_{n+1} - \theta_n - \Delta_\theta) a.$$ 

In the ordered phase for $|\Delta_\theta| < \frac{1}{2}$ all the $\theta_n$ take the same value in the ground state, so the angular pitch $Q_\theta$ is equal to zero. For $\frac{1}{2} < \Delta_\theta < \frac{3}{2}$ the angular pitch is equal to 1. There, the system is in its ground state close-packed with clockwise domain walls.

In the other low temperature limit $\beta \to -\infty$, the ordered phase for $0 < \Delta_\theta < 1$ has an angular pitch $Q_\theta = -1$.

In the high-temperature limit, $\beta \to 0$, where the Hamiltonian reduces to

$$H = -\sum_n \cos(\theta_n - \Delta_\theta) a,$$

there are two different disordered phases. They can be distinguished by the momentum pitch: for $|\Delta_\rho| < \frac{1}{2}$, $Q_\rho = 0$, while for $\frac{1}{2} < \Delta_\rho < \frac{3}{2}$, $Q_\rho = 1$.

In the incommensurate phases the pitches vary continuously. Figs. 3 and 4 show how we visualize this variation. In the incommensurate phases the correlation functions do not only have a continuously varying periodicity but also decay algebraically, with continuously varying critical indices. Fig. 5 shows schematically the lines in these phases along which the exponents will be constant.

Fig. 3. Dashed lines represent lines of constant momentum pitch.
Fig. 4 Dashed lines represent lines of constant angular pitch.

Fig. 5. Lines of constant critical indices in the incommensurate phase.
The reader might be surprised by the structure of the phase diagram at high temperatures. At $\beta = 0$ we find a phase transition between two disordered phases. In this case, the Hamiltonian

$$H_n = -\cos(p_n - \Delta_p)a$$

might be interpreted as describing a one-dimensional statistical mechanical model. In one dimension there are not supposed to be phase transitions. In appendix A we show that $\Delta_p$ actually leads to a classical model with complex coupling constants for the “time direction” bonds of the two-dimensional lattice. The phase transition at $\beta = 0$ is a result of choosing the lowest energy solution between two solutions which have different quantum numbers. This choice is naturally made by the system if we impose periodic boundary conditions.

2. Symmetries

This section describes the symmetries of the Hamiltonian, eq. (1.5). Consider $H$ as the sum of a kinetic energy term and an interaction: $H = H_0 + V$, with

$$H_0 = -\sum_n \cos(p_n - \Delta_p)a, \quad V = -\beta\sum_n \cos(\theta_{n+1} - \theta_n - \Delta_p)a.$$  \hspace{1cm} (2.1)

The coupling constant $\beta$ is proportional to the inverse temperature. The conjugate variables $\theta, p$ define ladder operators as follows:

$$e^{\pm i\theta_n} |p_n\rangle = |p_n \pm 1\rangle, \quad e^{\pm ip_n} |\theta_n\rangle = |\theta_n \mp 1\rangle.$$  \hspace{1cm} (2.2)

This is simply a restatement of the commutation relation (1.1).

The fact that $V$ depends only on the difference $\theta_{n+1} - \theta_n$ implies a conservation law, namely conservation of total momentum $P = \sum_n p_n \pmod{3}$. In other words, the $Z_3$, or clock symmetry of $V$ means that the eigenstates may be labelled by their value of $P$. Besides this “internal translation” invariance, the Hamiltonian is also translationally invariant in the usual sense, due to the definition of $H$ on a periodic lattice. We would then expect Bloch’s theorem to hold. Indeed, this has important consequences for the excited states, as explained in sect. 4.

Self-duality allows us to relate the high- and low-temperature properties of the model. If $\tilde{\eta}$ refers to the bond between sites $n$ and $n + 1$, the dual variables are defined as

$$\tilde{\theta}_{\tilde{n}} = \theta_{n+1} - \theta_n, \quad \tilde{\theta}_{\tilde{n}} = \sum_{m < n} p_m.$$ \hspace{1cm} (2.3)
This transformation preserves the commutation relation (1.1), and implies
\[ H(\beta, \Delta_\theta, \Delta_p; \theta_n, p_n) = \beta H(\beta^{-1}, \Delta_p, \Delta_\theta; \hat{\theta}_n, \hat{p}_n). \]  
(2.4)

For \( \beta > 0 \), this maps ground states at high temperature onto ground states at low temperature, and exchanges \( \Delta_\theta \) and \( \Delta_p \).

The important symmetries with respect to transformation of the misfit fields \( \Delta_\theta \) and \( \Delta_p \) are
\[ H(\beta, \Delta_\theta, \Delta_p; \theta_n, p_n) = H(\beta, -\Delta_\theta, -\Delta_p; -\theta_n, -p_n) \]  
(2.5a)
\[ = H(\beta, -\Delta_\theta, \Delta_p; -\theta_n, p_n) \]  
(2.5b)
\[ = H(\beta, \Delta_\theta + k, \Delta_p + j; \theta_n + kn, p_n + j). \]  
(2.5c)

Here, \( j \) and \( k \) are integers. In (2.5b) we refer to a system where the lattice sites are numbered from \(-N\) to \(N\). These symmetries imply that it is sufficient to study the region \( 0 \leq \Delta_p, \Delta_\theta < \frac{1}{4} \).

The phase diagram for \( \beta < 0 \) refers to a system with antiferromagnetic couplings in the space direction. By combining (2.3)–(2.5), the form of self-duality relevant for \( \beta < 0 \) is
\[ H(\beta, \Delta_\theta, \Delta_p; \theta_n, p_n) = -\beta H(\beta^{-1}, -\frac{1}{2} - \Delta_p, -\frac{1}{2} - \Delta_\theta; \theta_n', p_n') \]
\[ \theta_n' = \sum_{m < n} 1 + p_m, \quad p_n' = \theta_{n+1} - \theta_n - 1. \]  
(2.6)

The Lifshitz points are located at \( \Delta_\theta = \Delta_p = \frac{1}{4} \), \( \beta = \pm 1 \). Special symmetries apply here which make these points especially important. The transformation \( p_n' = p_{-n}, \theta_n' = \theta_{-n} + n \) leads to the symmetry relation
\[ H(\beta, \Delta_\theta, \Delta_p; \theta_n, p_n) = H(-\beta, \frac{1}{4} - \Delta_\theta, \frac{1}{4} - \Delta_p; \theta_n', p_n'), \]  
(2.7)
so at \( \Delta_\theta = \Delta_p = \frac{1}{4} \), the ground-state energy is an even function of \( \beta \). We conclude that the critical indices at the two Lifshitz points are identical, although the pattern of lines emerging from them is different.

3. Series expansions

3.1. Outline of Method

The eigenvalues of a quantum hamiltonian give information about the associated 2D model. In particular, the ground-state energy of \( H \) is the free energy, and the
mass gap (difference between the first excited and ground-state energies) is the inverse correlation length. Details of the correspondences may be found in Kogut's review article [2].

Suppose one has a perturbation expansion for an eigenvalue:

\[ e(\beta, \Delta) = \sum_{n=0}^{M} e_n(\Delta) \beta^n + O(\beta^{M+1}) \]  

If \( e(\beta, \Delta) \) exhibits an algebraic singularity at some critical coupling constant, \( \beta_c \), i.e., \( e(\beta, \Delta) \sim (\beta_c - \beta)^b \) as \( \beta \to \beta_c \), then both \( \beta_c \) and \( b \) may be computed using standard series method, e.g., Diog Padé. In cases where \( \beta_c \) is not small, it is necessary to have rather long series in order to extract reliable estimates of \( \beta_c \) and \( b \). We have used the connected diagram perturbation method of Kadanoff and Kohmoto [5]; it is particularly suited to calculating the higher order expansion terms.

The unperturbed ground state of \( H \) is the vacuum

\[ |\psi\rangle_{\beta=0} = |p_n = 0, n = 1, 2, \ldots \rangle, \quad 0 < \Delta < \frac{1}{2}. \]  

The specific heat is obtained from the ground-state energy series by differentiation:

\[ C(\beta, \Delta) = \frac{\partial^2}{\partial \beta^2} E_0(\beta, \Delta). \]  

To calculate the ground-state expectation value of an operator \( O = \sum a_{Q_n} \), simply add a magnetic field term to \( H \), i.e., \( H \rightarrow H + hO \), and calculate the ground-state energy in the presence of \( h \). The expectation value is then given by

\[ \langle O \rangle = \frac{\partial E_0(h)}{\partial h} \bigg|_{h=0}, \]  

and the susceptibility is

\[ \langle O^2 \rangle - \langle O \rangle^2 = \frac{\partial^2 E_0(h)}{\partial h^2} \bigg|_{h=0}. \]  

If one performs a small \( \beta \) (high temperature) expansion, it is convenient to calculate the expectation value of the disorder operator,

\[ D = \sum_n \cos \left( a \sum_{m \leq n} p_m \right). \]  

This operator is dual to the usual order operator, or magnetization, and so

\[ \langle D \rangle_\beta = \left( \sum_n \cos \theta_n a \right)_\beta. \]
Recall from sect. 2 that the $Z_3$ symmetry of $H$ implies that the eigenstates have a
definite total momentum equal to 0, 1 or 2. For $0 \leq \Delta_p < \frac{1}{2}$ the first excited state of
the unperturbed Hamiltonian lies in the $P = 1$ sector, and consists of a single site
with non-zero momentum. In addition, the excited state is labelled by a wave vector,
$q$:

$$|\psi_i\rangle_{\beta=0} = \sum_n |p_n = 1, p_{m+n} = 0\rangle e^{-i\alpha n q}, \quad |q| \leq \frac{3}{2}.$$  \hspace{1cm} (3.8)

The plane-wave modulation is a consequence of Bloch's theorem. Note that the mass
gap, $m$, will depend on the continuous parameter $q$.

To see the implications of the $q$-dependence, consider the first order mass gap:

$$m^1 = \cos(a\Delta_p) - \cos(\Delta_p - 1)a - \beta \cos(\Delta_\theta - q)a.$$  \hspace{1cm} (3.9)

If there is a phase transition for $\beta_c \ll 1$, the value of $\beta_c$ may be obtained by requiring
$m^1$ to vanish:

$$\beta_c = \frac{\cos(a\Delta_p) - \cos(\Delta_p - 1)a}{\cos(\Delta_\theta - q)a}.$$  \hspace{1cm} (3.10)

Of course, if $\Delta_p = 0$, there is no crossing of eigenvalues for small $\beta$. In our self-dual
model, with $\Delta_p = \Delta_\theta \sim \frac{3}{2}$, the C-I line extends to $\beta = 0$ (cf. fig. 2). For fixed $\Delta_p$, $\Delta_\theta$, the value of $q$ which minimizes $\beta_c$ defines the critical wavevector, $q_c$. According to
(3.10), $q_c = \Delta_\theta$ for $\beta_c > 0$ and $q_c = \Delta_\theta - \frac{3}{2}$ for $\beta_c < 0$. This suggests that along the
entire commensurate-incommensurate line $q_c$ varies continuously with $\Delta_\theta$. In fact, $q_c$
is equal to the value of the angular pitch at the C-I phase boundary (see fig. 4).

However, as $\beta_c$ increases the $q$-dependence must be deduced from the series for $m$.
First, we locate the minimum $\beta_c$ by examining the gap for various values of $q$:

$$\beta_c(\Delta) = \min(\beta: m(\beta, \Delta, q) = 0, |q| \leq \frac{3}{2}),$$

$$\Delta = \Delta_\theta = \Delta_p.$$  \hspace{1cm} (3.11)

The critical wave vector is then defined by

$$m(\beta_c(\Delta), \Delta, q_c(\Delta)) = 0.$$  \hspace{1cm} (3.12)

Figs. 10 and 11 display the $\Delta$ dependence of $q_c$. The interpretation of $q$ in terms of
the free-fermion approximation is presented in sect. 4.

The method outlined in this section is restricted to the calculation of single-excitation mass gaps. In the case of C-I transitions, this is sufficient if the transition is second order, i.e. the number of domain walls increases continuously from zero. If
the transition is first order, it would be necessary to calculate all types of multi-excitation mass gaps, and to determine which one vanishes first.

3.2 RESULTS FROM SERIES ANALYSIS

We have used strong coupling expansions to determine critical points and critical indices. Specifically, we have generated:

(a) Thirteenth order series for the ground-state energy, magnetization and susceptibility.

(b) Ninth order series for the \( q \)-dependent mass gap.

Critical points and indices are found by the Dlog Padé method. The best estimate for a quantity is obtained by averaging the three or four highest order diagonal and near-diagonal entries of the Padé table. Error bars are then set to include all three or four values.

3.2.1. Lifshitz Points, \( \Delta = \frac{1}{4}, \beta = \pm 1 \). Our interpretation of the series analysis is, to a large extent, guided by the rather remarkable results obtained at \( \Delta = \frac{1}{4} \). According to eq. (2.7) the ground-state energy, magnetization, and susceptibility are even functions of \( \beta \) at \( \Delta = \frac{1}{4} \). One surprising result is that the magnetization appears to be exactly represented as

\[ \langle D \rangle = (1 - \beta^2)^{1/9}. \]  

This is suggested by the fact that our series for \( \langle D \rangle \) reproduces the binomial expansion of (3.13) to thirteenth order. Eq. (3.13) exhibits the critical index which has been conjectured for the three-state Potts model, namely \( \beta = \frac{1}{4} \) [6].

The specific heat and susceptibility series also imply \( \beta_c = \pm 1 \); the critical indices \( \alpha \) and \( \gamma \) are found to be

\[ \alpha = 0.374 \pm 0.003, \quad (0.333 \ldots), \]  
\[ \gamma = 1.48 \pm 0.02, \quad (1.444 \ldots). \]

The values in parentheses are the conjectured exact results for the three-state Potts model [6, 14].

On the other hand, the mass gap series also suggest an exact result; all the coefficients beyond first order are zero (up to tenth order), and so

\[ m(q = 0) = \frac{1}{2} \sqrt{3} (1 - \beta), \]  

and

\[ m(q = -1) = \frac{1}{2} \sqrt{3} (1 + \beta). \]
The mass gap index, \( \nu \), thus appears to be exactly given by

\[
\nu(\Delta = \frac{1}{2}) = 1,
\]

characteristic of the Ising model. Eqs. (3.14a) and (3.14b) violate the hyperscaling relation \( \alpha = 2 - 2\nu \). However, this is perhaps tolerable if we believe that \( (\beta = 1, \Delta = \frac{1}{2}) \) is a particularly singular point on the phase diagram, namely the point at which the two C-I lines meet the Potts line. The critical properties at \( \beta = -1 \) are different only insofar as \( q_c = -1 \), reflecting the fact that the angular pitch in the \( \beta \to -\infty \) phase is also given by \( Q_\theta = -1 \). As well, this Lifshitz point is the intersection of four C-I lines. In the model studied by Ostlund \( (\Delta_P = 0) \), the Lifshitz point is presumed to be the intersection of a C-I line, a Potts line, and a Kosterlitz-Thouless line (cf. fig. 1). We are currently investigating the possibility that this model exhibits the same peculiar behavior at its Lifshitz point.

Note that the mass gaps (3.15) are obtained perturbatively from (3.8), which is the lowest excited state of \( H_0 \). The mass corresponding to the next highest excitation, namely

\[
|\psi_2\rangle_{\beta = 0} = \sum_n |p_n = 2, p_{m+n} = 0\rangle e^{-i\alpha q},
\]

should either lie above the lowest excitation mass, or vanish at the same \( \beta_c \) with the same critical index. Unfortunately, at \( \Delta = \frac{1}{4} \), the kinetic energies of the excitations \( p = 0, 1, 2 \) are evenly spaced, and so the state (3.17) is degenerate with the "two-particle" state

\[
|\psi_1\rangle_{\beta = 0} = \sum_n |p_n = p_{n+1} = 1, p_{m+n, n+1} = 0\rangle e^{-i\alpha q}.
\]

We cannot use our perturbation scheme to calculate the mass corresponding to either (3.17) or (3.18), but the results on the Potts line suggest that the mass of the state with total momentum \( P = 2 \) (which could be calculated using degenerate perturbation theory) vanishes linearly, at \( \Delta = \frac{1}{4} \).

3.2.2. Potts line, \( \beta > 0, 0 \leq \Delta < \frac{1}{4} \). Based on the results at \( \Delta = \frac{1}{4} \), one expects three-state Potts behaviour for \( 0 \leq \Delta < \frac{1}{4} \), i.e., \( \beta_c = 1 \), and constant critical indices. Also, if the Potts permutation symmetry is unbroken the masses \( m_1 \) and \( m_2 \), corresponding to (3.8) and (3.17) respectively, should both vanish at \( \beta_c = 1 \) with the same value of \( \nu \). Indeed, all series consistently predict a \( \beta_c \) very nearly equal to one, so to improve the accuracy of the indices, we have assumed \( \beta_c = 1 \) along this line.

The indices \( \alpha, \beta, \) and \( \gamma \) are shown in figs. 6–8. Although the data lie beyond the exact Potts values, there is a definite improvement as \( \Delta \) approaches the Lifshitz point. This leads us to believe that the variation is a result of using finite series, or perhaps due to competing singularities. Further evidence that the Potts symmetry is
Fig. 6  Specific heat index along the Potts line.

Fig. 7  Magnetization index along the Potts line.

Fig. 8  Susceptibility index along the Potts line.
unbroken comes from the critical wave vector, \( q_c \). At \( \Delta = 0 \), \( q_c = 0 \), so to check that this remains true, we examine mass gaps \( m(q) \) for \( q \) approximately zero, and compare \( \beta_c(q) \) with \( \beta_c(0) = 1 \). For \( |q| > 0.01 \), \( \beta_c(q) > 1 \), and so we conclude

\[
q_c(\Delta) = 0 \pm 0.01, \quad 0 \leq \Delta < \frac{1}{4}.
\]

(3.19)

The mass gap indices \( \nu_1 \) and \( \nu_2 \), for \( m_1(q = 0) \) and \( m_2(q = 0) \) respectively, are shown in fig. 9. We find that \( \nu_1 \) rises steadily from its value at \( \Delta = 0 \),

\[
\nu_1(0) = 0.838 \pm 0.002, \quad \text{(exact: 0.833...)},
\]

(3.20)

to the value which we believe is true at \( \Delta = \frac{1}{4} \), \( \nu_1(\frac{1}{4}) = 1 \). On the other hand, \( \nu_2 \) is quite stable for \( 0 \leq \Delta \leq 0.10 \), and then appears also to approach the value one at \( \Delta = \frac{1}{4} \). This suggests that an exact or higher order calculation would predict a constant \( \nu_2 \). Our results cannot rule out the rather unpalatable conclusion that \( \nu_1 \) varies continuously along this line, but this may not occur in a different approximation scheme.

3.2.3. Commensurate-incommensurate lines

(a) \( \beta > 0 \).

The free-fermion approximation of sect. 4 predicts a C-I critical line which extends from the point \( (\beta = 0, \Delta = \frac{1}{4}) \) with a slope of \( -2\pi/\sqrt{3} \). The same analysis indicates that the free energy is non-singular as the C-I line is approached from the commensurate side. Therefore, only the mass gap is useful for determining the phase boundary. Henceforth, we shall only refer to \( m_1 \), the mass of the \( P = 1 \) state; along the C-I lines, the other mass, \( m_2 \), appears to always lie above \( m_1 \). Using the method outlined in subsect. 3.1, we find, at \( \Delta = 0.49 \),

\[
q_c = \Delta + O(\beta^2),
\]

\[
\beta_c = \frac{2\pi}{\sqrt{3}} (\frac{1}{4} - \Delta) + O(\beta^2),
\]

\[
\nu = 1 + O(\beta^2),
\]

(3.21)

![Fig. 9 Mass gap indices for the \( \beta > 0 \) critical line](image-url)
which agrees with the free-fermion approximation. The series for the specific heat, magnetization and susceptibility suggest $\beta_c(\Delta = 0.49) = 0.09; (2\sqrt{\frac{1}{3}} \pi \times 0.01 = 0.04)$, but the critical indices at this $\beta_c$ are either very small, in comparison with the Potts value, or quite erratic. This behaviour is consistent with the fermion model prediction that there is no singularity in these quantities for $\beta \leq \beta_c$. Hence, the observed "singularity" can be regarded as merely an unphysical consequence of pushing the Padé approximation scheme too far.

Repeating this procedure along the C-I line from $\Delta = \frac{1}{2}$ to $\Delta = \frac{1}{4}$, we find the critical points as indicated in fig. 2, the critical wave vector as a function of $\Delta$ in fig. 10, and the mass gap exponent $\nu$ in fig. 9. The other three series continue to predict values of $\beta_c$ which are greater than the one deduced from the mass gap. This, combined with the erratic behavior of $\alpha, \beta$ and $\gamma$ leads us to believe that the free-fermion picture of the C-I transition is true even near the Lifshitz point--$q_c$ varies continuously, and the mass gap vanishes linearly.

(b) $\beta < 0$.

The free-fermion predictions also apply to the critical line for $\beta < 0$ extending from ($\beta = 0, \Delta = \frac{1}{2}$) with slope $2\pi/\sqrt{3}$, namely line C'D of fig. 2. Along this line, we find results similar to the ones described in part (a). Fig. 11 shows that $q_c$ varies continuously, but now exhibits a minimum at $\Delta = 0.35$. The mass gap index along

![Fig 10. Critical wavevector for the $\beta > 0$ critical line](image1)

![Fig 11 Critical wavevector for the $\beta < 0$ critical line.](image2)
C'D, in fig. 12, is quite close to its free-fermion value. Note in fig. 2 that GD has been labelled a C-I line. This follows from the analysis of sect. 5. The data for line ED (which is dual to line GD) tend to support this idea, but the mass gap series is rather unstable here. Results for \( q_c \) and \( \nu \) are shown in figs. 11 and 12, respectively.

3.2.4. Kosterlitz-Thouless transitions. The Hamiltonian (1.5) with \( \Delta_p = \Delta_\beta = 0 \) and \( \beta < 0 \) describes the three-state Potts model with antiferromagnetic couplings in the space direction. According to (2.6), the line \( (\beta < 0, A = 0) \) is dual to the line \( (\beta^{-1} < 0, \Delta = \frac{1}{2}) \). We know from the free-fermion approximation that a floating phase exists at \( \Delta = 0 \) for large negative \( \beta \). However, we expect the floating phase to melt to a high-temperature commensurate phase via the unbinding of dislocation pairs (cf. subsect. 5.3). To find the critical point for this transition we have examined the series at \( \Delta = 0 \), along the negative \( \beta \) axis. Since the thermodynamic quantities are expected to exhibit an essential singularity, the standard Dlog Padé method is inadequate. Instead, we have used a technique proposed by Rehr [7] which is basically a ratio test for functions with an essential singularity. The technique has not yet been fully exploited by us, so we shall only report preliminary results. The susceptibility, which diverges as

\[
\chi \sim \epsilon^{A(\beta - \beta_c)^{-\epsilon}}, \quad A, \sigma > 0,
\]

is the best-behaved series. If we assume \( \sigma = \frac{1}{2} \), as in the Kosterlitz-Thouless theory, the evidence suggests that

\[
\beta_c(\Delta = 0) = -10 \pm 5.
\]

This implies that at \( \Delta = \frac{1}{2} \), the incommensurate phase melts at \( \beta_c(\frac{1}{2}) \approx -0.10 \) although perhaps the best estimate for \( \beta_c(0) \) is obtained by extrapolating line ED of fig. 2 to \( \Delta = 0 \).
4. The fermion approach

4.1. THE METHOD

In this section we will describe a systematic method to obtain an effective spin-$\frac{1}{2}$ hamiltonian for our model. This is obtained as an expansion around the point $C'$ in fig. 2 (and C, F and F') which is carried out up to second order in $\beta$ (or $\beta^{-1}$).

To order $\beta$, the system reduces to a free fermion model. The idea of treating the meandering of a system of domain walls with a hard core by a one-dimensional free fermion model originates with De Gennes [8]. More recently it was applied by Villain and Bak [9] to the ANNNI model, and by Osthund [1] to the asymmetrical clock model, which differs from ours in that it has no $\Delta$ in the kinetic energy term. These authors obtain the free fermion model directly from the 2-dimensional system. In our hamiltonian formalism one can see how to carry out this expansion in a systematic way, to arbitrary order.

Consider the hamiltonian (1.5) at $\beta = 0$:

$$H_0 = -\sum_n \cos(p_n - \Delta_p) a_n.$$  \hspace{1cm} (4.1)

By duality, $H_0$ also describes the model at $\beta = \infty$, where we replace $p_n$ by $\theta_{n+1} - \theta_n$. There, the analog of $p_n = 0$ corresponds to a situation in which two neighbouring $\theta$'s are equal, i.e., there is no domain wall at $n + \frac{1}{2}$. Then, the analogs of $p_n = +1$ and $p_n = -1$ represent respectively domain walls for which $\theta$ rotates as $n$ is increased through one unit in the clockwise or counterclockwise directions. At $\Delta_p = \frac{1}{2}$ the energies of $p = 0$ and $p = +1$ become equal. The ground state is infinitely degenerate, since clockwise domain walls can be placed at random. Our Rayleigh-Schrödinger perturbation expansion fails.

To make further progress, we must switch from ordinary perturbation theory to degenerate state perturbation theory. To do this, we use as our basis the set of states with $p = 0$ and $p = +1$ and treat the $p = -1$ states as a perturbation. The latter states are called impurity states since they provide scattering centers analogous to impurities in the fermion model which will be written down in the next few paragraphs.

To derive the fermion approach it is best to think of the three state model as representing a spin-1 system, with $\sigma^z_n$ taking on the values $(0, +1, -1)$ corresponding respectively to $p_n = (-1, +1, 0)$. As $\Delta_p \rightarrow \frac{1}{2}$ the latter two states are almost degenerate, while the first, $\sigma^z = 0$, lies higher and is mostly "frozen out". We should then rewrite the hamiltonian in the form of a sum of terms, one of which produces motion within the $\sigma^z = \pm 1$ space and the other which moves one into or out of that space. This is done simply by taking

$$H_0 = \sum_n \frac{1}{2} \mu \sigma^z_n + g(1 - (\sigma^z_n)^2)$$  \hspace{1cm} (4.2)
with the chemical potential, $\mu$, and the impurity gap $g$ being given by

$$\mu = - \left[ \cos(1 - \Delta_p) a - \cos(a \Delta_p) \right], \quad (4.3)$$

$$g = - \cos(1 + \Delta_p) a + \frac{1}{2} \left[ \cos(1 - \Delta_p) a + \cos(a \Delta_p) \right]. \quad (4.4)$$

Around $\Delta_p = \frac{1}{2}$, $\mu$ is proportional to $(\frac{1}{2} - \Delta_p)$ and the impurities are frozen out because $g = \frac{1}{2}$ is much larger than $\mu$.

We now seek an effective Hamiltonian which acts fully within the “pure” space $\sigma^z = \pm 1$. In this space define operators $\sigma^z$ by $\sigma^z | \pm 1 \rangle = | \pm 1 \rangle$. Then one can write the potential term as

$$V = -\beta \sum_n \cos(\theta_{n+1} - \theta_n - \Delta_\theta) a$$

$$= W_1 + V_1. \quad (4.5)$$

Here $W_1$ is the part of $V$ which only connects states within the pure space:

$$W_1 = -\frac{1}{2} \beta \sum_n \sigma_n^z \sigma_{n+1}^z e^{ia\Delta_\theta} + \sigma_n^+ \sigma_{n+1}^- e^{-ia\Delta_\theta}. \quad (4.6)$$

The remaining piece $V_1$ creates impurities when applied to a state of the $\sigma^z = \pm 1$ subspace. The effects of $V_1$ can be treated perturbatively because $g$ is large with respect to $\beta$ and $\Delta_p - \frac{1}{2}$.

To order $\beta$, $V_1$ does not contribute:

$$\langle a | V_1 | b \rangle = 0 \quad (4.7)$$

with $|a\rangle$ and $|b\rangle$ states in the $\sigma^z = \pm 1$ subspace. So

$$H_1 = H_0 + W_1 \quad (4.8)$$

is exact up to order $\beta$. Let $|a^{(1)}\rangle$ and $|b^{(1)}\rangle$ be eigenstates of $H_1$. The second order effects of $V_1$ can be represented by an effective operator $W_2$, which is defined as

$$\langle a^{(1)} | W_2 | b^{(1)} \rangle = \langle a^{(1)} | V_1 (H_1 - E_b^{(1)})^{-1} V_1 | b^{(1)} \rangle. \quad (4.9)$$

If we introduce $H_2$ and $V_2$ as

$$H_2 = H_1 + W_2, \quad (4.10)$$

$$V_2 = V_1 - W_2, \quad (4.11)$$
then $V_2$ only introduces effects of order $\beta^3$, and $H_2$ is an effective spin-$\frac{1}{2}$ hamiltonian which is exact up to order $\beta^2$.

We will find that $H_2$ is a model of interacting fermions, similar to the $XXZ$ model [10, 11]. It is well known how to obtain a continuum formulation for such a model (see refs. [12–15]). From that the critical properties of the floating phases in fig. 2 will be obtained.

First we will discuss the free fermion model $H_1$ and review its properties that justify the identification of its massless phase with an incommensurate floating phase.

### 4.2 THE FREE FERMION MODEL

To order $\beta$, the effective hamiltonian becomes a free fermion model:

$$H_1 = \sum_n \frac{1}{2} \mu \sigma^z_n - \frac{1}{2} \beta \left( \sigma^+_n \sigma^-_{n+1} e^{ia\Delta_x} + \sigma^-_n \sigma^+_{n+1} e^{-ia\Delta_x} \right), \quad (4.12)$$

with $\sigma^z_n = \pm 1$. (At this point, impurity states $\sigma^z_n = 0$ are ignored since the sector without impurities contains the ground state and lowest excitations.) After a Jordan-Wigner transformation to fermion variables, which anticommute at different sites,

$$\sigma^+_n = a^+_n \exp \left( i \pi \sum_{m=1}^{n-1} a^+_m a_m \right), \quad (4.13)$$

followed by a Fourier transformation

$$a^+_n = \sum_k a^+ (k) e^{ikn}, \quad (4.14)$$

the hamiltonian becomes diagonal:

$$H_1 = \sum_k \left[ \mu - \beta \cos (k - a\Delta_x) \right] a^+ (k) a (k). \quad (4.15)$$

Let us review the main properties of this hamiltonian. $\mu$ is the energy needed to create a domain wall. The cosine term represents its “thermal” meandering energy. The fermions can freely hop from site to site with probability $\beta$, and are only restricted by the Pauli exclusion principle.

The energy needed to create a fermion outweighs the gain in meandering energy for $\mu > \beta$. For $-\beta < \mu < \beta$ the number of fermions increases continuously. For $\mu < -\beta$ there is a domain wall at each site. The ground state is obtained by filling the band up to the Fermi surface.
The average number of domain walls, which is identical to the momentum pitch \( Q_p \) (see introduction), varies as

\[
Q_p = \langle 0| a_{a_n}^\dagger a_n |0\rangle = \frac{k_F^{(+)r} - k_F^{(-)l}}{2\pi} = \frac{1}{\pi} \cos^{-1}(\mu/\beta),
\]

(4.16)

when \( |\mu| < \beta \) and is zero for \( |\mu| > \beta \) (see fig. 13).

So indeed \( Q_p \) varies continuously in the floating phase and takes irrational values which are incommensurate with the lattice. The empty \( (Q_p = 0) \) and full \( (Q_p = 1) \) phases at \( \mu > \beta \) and \( \mu < -\beta \) are commensurate. The C-I transition lines are located at \( \mu = \beta \), i.e., \( \beta = \pm 2\sqrt{\frac{1}{2} \pi (\frac{1}{2} - \Delta_p)} \).

Another characteristic of the incommensurate phase is its critical nature. The mass gap (the energy needed to put in an extra fermion) is zero (i.e., it vanishes in the thermodynamic limit as \( 1/N \)). Since the correlation functions decay as a power law, one describes the phase as a gaussian or floating phase. For example, the density-density correlation function behaves as

\[
\langle 0| a_{a_n}^\dagger a_n a_{a_{n+1}}^\dagger a_{a_{n+1}} |0\rangle = \frac{\sin^2(\pi r Q_p)}{(\pi r)^2} + Q_p^2.
\]

(4.17)

The fluctuations around the mean number of domain walls \( Q_p \) are large, and the correlation function oscillates. The domain walls form a "lattice" with lattice constant \( 1/Q_p \). This lattice structure is induced by the thermal meandering energy. Only at \( (\beta = 0, \Delta_p = \frac{1}{2}) \) are the domain walls placed at random.

The pitch \( Q_p \) goes to zero at the C-I phase boundary with a critical exponent \( \beta = \frac{1}{2} \) [see eq. (4.16)]. This value is universal, and independent of details of the shape of the dispersion relation. It is a direct result of the quadratic shape of the bottom of the band.

![Diagram](image.png)

Fig. 13 Free-fermion dispersion relation for \( \beta > 0 \). For \( \beta < 0 \) the minimum is located at \( k = \Delta a - \pi \).
The specific heat exponent $\alpha$ is given by $\alpha = \frac{1}{2}$. To see this notice that the ground-state energy behaves as

$$E_0 \sim \int_0^\beta |x - \mu|^{1/2} \, dx \sim \beta - \mu^{2 - \alpha} \quad (4.18)$$

in the floating phase. As one approaches the phase transition from the commensurate side where there are no fermions, $E_0$ appears to be regular.

Recall from the introduction our definition of the two pitches in terms of the periodicity in the long-range behaviour of correlation functions. For small $\beta$ we argued that the momentum pitch can also be defined via the expectation value of a local operator, i.e., as the density of fermions. Similarly, the angular pitch becomes equivalent to the average value of the momenta $k$, which label the occupied, single fermion eigenstates:

$$Q_\theta = \frac{k_F^{(+)} + k_F^{(-)}}{2\pi} \quad (4.20)$$

We can verify this by calculating the correlation functions (1.2) and (1.6) in the fermion approximation. The long-range behaviour is easily found by the continuum limit methods (see appendix B and also refs. [12-15]) to be

$$\langle 0 | \exp \left( i a \sum_{n-k}^{j-1} p_n \right) | 0 \rangle = \langle 0 | \exp \left( i a \sum_{n-k}^{j-1} a_n^+ a_n \right) | 0 \rangle \sim \frac{1}{|j - k|^{2/9}} e^{i a Q_\theta (j-k)} \quad (4.21)$$

$$\langle 0 | \exp ia (\theta_j - \theta_k) | 0 \rangle = \langle 0 | a_j^+ \exp \left( i \pi \sum_{n=k}^{j-1} a_n^+ a_n \right) a_k | 0 \rangle \sim \frac{1}{|j - k|^{1/2}} e^{i a Q_\theta (j-k)} \quad (4.22)$$

where $Q_\mu$ and $Q_\theta$ indeed take the values quoted in eqs. (4.16) and (4.20).

Let us finish with some comments about the series calculation (compare with sect. 3). We have seen here that the C-I transition is the result of a crossing of eigenvalues. A series expansion from the commensurate side for the ground-state energy cannot predict such a transition. It analytically continues the eigenvector which is the wrong ansatz at the incommensurate side. There is no reason to expect a singularity in the eigenvalues at the moment of crossing.

In sect. 3 it is explained how the C-I transition line is obtained from the series of the mass gap $m(q)$. In terms of the free fermion model the interpretation of $m(q)$ is simple: it is the energy it costs to create a single fermion in the band at wave number $k = qa$. The C-I transition occurs at the moment $m(\Delta q)$ vanishes, because $q = \Delta q$ corresponds to the bottom of the band. For $\beta < 0$ the minimum is at $q = \Delta q - \frac{1}{2}$. 
4.3. THE EFFECTIVE HAMILTONIAN TO ORDER $\beta^2$

Fig. 14 shows the diagrams which determine the effective second-order operator $W_2$ [see eq. (4.9)].

The notation of the diagrams is as follows: A solid line represents a domain wall ($p_n = +1$) and a dashed line an impurity ($p_n = -1$). The horizontal lines represent the action of the potential operator $V_1$ [see eq. (4.5)]. The arrows account for the sign of the phase factor $e^{\pm ia\Delta}$. In diagram (d), for example, one starts with no domain walls at three neighbouring sites. In the first time step a domain wall and an impurity are created. In the second step the impurity is destroyed and replaced by two domain walls. One is back in the spin-$\frac{1}{2}$ subspace. The effective operator for this process is $(\beta^2/4g)\sigma_+\sigma_{+1}\sigma_+\sigma_{+2}$ which creates three domain walls at once. There is no net phase factor, because the two arrows point in different directions. It is by this process that the system remembers that it is back at the same value of $\theta$ after three clockwise domain walls.

The complete form of $W_2$ reads

$$W_2 = - (\frac{1}{4} \beta)^2 \sum \frac{1}{4g} (3\sigma_+^\dagger \sigma_{+1}^\dagger + 5) + \frac{2}{g} (\sigma_+^\dagger \sigma_{+1}^\dagger \sigma_{+2}^\dagger + \text{h.c.})$$

$$+ \frac{2}{g} (\sigma_+^\dagger \sigma_{-1}^\dagger e^{-2ia\Delta} + \text{h.c.}) + \frac{1}{g} (\sigma_+^\dagger \sigma_{+2}^\dagger e^{2ia\Delta} + \text{h.c.}). \tag{4.23}$$

The first term is a nearest-neighbour interaction between domain walls and originates from the difference between the number of impurities in the intermediate state of the diagrams (a), (b), and (c) and also because (a) and (c) occur twice, while (b) only once. Notice the sign: domain walls attract each other. The dislocation operator

\begin{align*}
\begin{array}{c}
\text{(a)} \\
\frac{1}{2g} \\
\frac{1}{g} \\
\end{array} & \quad \begin{array}{c}
\text{(b)} \\
\frac{1}{2} \\
\frac{1}{3} \\
\end{array} & \quad \begin{array}{c}
\text{(c)} \\
\frac{1}{2} \\
\frac{1}{3} \\
\end{array} \\
\begin{array}{c}
\text{(d)} \\
\frac{1}{2} \\
\frac{1}{3} \\
\end{array} & \quad \begin{array}{c}
\text{(e)} \\
\frac{1}{3} \\
\frac{1}{2} \\
\end{array} \\
\begin{array}{c}
\text{(f)} \\
\frac{1}{2g} \\
\frac{1}{2} \\
\end{array} & \quad \begin{array}{c}
\text{(g)} \\
\frac{1}{2} \\
\frac{1}{3} \\
\end{array} & \quad \begin{array}{c}
\text{(h)} \\
\frac{1}{2g} \\
\frac{1}{3} \\
\end{array}
\end{align*}

Fig. 14. Second-order diagrams for the effective spin-$\frac{1}{2}$ hamiltonian
results from diagrams (d) and (e). Diagram (f) gives a nearest-neighbour hopping contribution, and diagrams (g) and (h) lead to the next-nearest-neighbour hopping interaction.

We have approximated in all these terms the resolvent \((H_1 - E_0^{(1)})^{-1}\) in eq. (4.9) by the impurity gap \(1/g\). This neglects the bandwidth of the free fermion model \(H_1\), but because \(g \gg \beta\) this is only a mistake that shows up in order \(\beta^3\).

5. Properties of the floating phases and the nature of their phase boundaries

5.1 RENORMALIZATION TRANSFORMATIONS

In the previous section we obtained an effective spin-\(1/2\) hamiltonian for our clock model in an expansion around the point \(C^\prime\) in fig. 2. By duality, it also applies to \(C\), \(F\) and \(F^\prime\). We will now deduce the general shape and the critical properties of the floating incommensurate phases in fig. 2.

In sect. 4 we discussed the properties up to order \(\beta\), which defines the free fermion model. The effects of the higher order contributions \(W_n\) (see subsects. 4.1, 4.3) can be studied by using operator product expansions like the ones used by Kadanoff et al. [16–19], or by studying the approach to a continuum limit [12–15]. In the continuum limit, our model maps into a generalized Thirring model, and then, after bosonization, into a generalized sine-Gordon model. One can recognize this last model in two-dimensional language as the continuum limit for a clock model with a real misfit parameter \(\Delta\) in one space direction and a pure imaginary one in the other direction.

The derivation of the continuum limit model is somewhat lengthy, so we shall present a "poor man's" way of obtaining in essence the same result, and leave the more formal and careful derivation for appendix B. This simplified derivation is related to the method introduced by José et al. [20] for the 2d clock models (without misfit fields). Knops [21] used it for the 6-vertex model, and Cardy [22] applied it recently to the 2d version of Ostlund's model.

Consider the hamiltonian of eq. (1.5). Replace the discrete spectra of the momentum and angle operators by continuous ones. The new operators \(-\infty < p < \infty\) and \(-\infty < \phi < \infty\) satisfy the canonical commutation relation \([\phi, p] = i\). The hamiltonian

\[
H = -\sum_n \beta \cos(\phi_{n+1} - \phi_n) + \cos(ap_n) \\
+ \beta y_\phi \cos(3\phi_n + 2\pi n \Delta_\phi) + y_\chi \cos(2\pi \sum_{m=-1}^n (p_m + n\Delta_\phi))
\]

reduces to the original one in the limit where the fugacities \(y_\phi\) and \(y_\chi\) go to infinity. These two extra operators take care of the spinwave and vortex excitations. There-
fore, one expects that for qualitative purposes one may expand the first two cosine terms and replace them by gaussians:

\[ H \approx \sum_n \frac{1}{2} \delta (\phi_{n+1} - \phi_n)^2 + \frac{1}{2} a^2 p_n^2 \]

\[ -\beta \gamma \cos(3\phi_n + 2\pi n \Delta_\phi) - \gamma \cos(2\pi \sum_{m=1}^n p_m + 2\pi n \Delta_p) . \] (5.2)

Our assertion is that the two hamiltonians (5.1) and (5.2) lie in the same universality class, i.e., they generate the same long distance correlations for \( e^{\pm i\phi_s} \) and \( \exp(\pm i\sum_{m=1}^n p_m) \) whenever the new parameter set \((\tilde{\beta}, \tilde{\Delta}_\phi, \tilde{\Delta}_p, \tilde{\gamma}_s, \tilde{\gamma}_v)\) is chosen to be appropriate functions of \( \beta, \Delta_\phi, \Delta_p, \gamma_s, \gamma_v \). (Of course, a major portion of our analysis will be the determination of how one set of parameters depend upon the others.) In fact, we have in mind a renormalization calculation (like that described for example in José et al. [20]) in which one gradually eliminates the spin wave and vortex excitations generated by \( \gamma_s \) and \( \gamma_v \). As this renormalization group calculation is carried out, all the parameters \( \mathbf{K} = (\tilde{\beta}, \tilde{\Delta}_\phi, \tilde{\Delta}_p, \tilde{\gamma}_s, \tilde{\gamma}_v) \) become functions of a single rescaling parameter, \( l \). In the incommensurate phase, as \( l \to \infty \), the vortex and spin wave excitations disappear so that \( \mathbf{K}(l) \to (K(\infty), \tilde{\Delta}_\phi(\infty), \tilde{\Delta}_p(\infty), 0, 0) \). If the hamiltonian eventually renormalizes to one with this structure, one calculates from the hamiltonian of eq. (5.2) expressions for the correlation functions \( C_p \) and \( C_\phi \), which are exactly of the form \((1.4)\) and \((1.6)\), i.e.,

\[ C_\phi(j - k) = \frac{A}{|j - k| \sqrt{K(\infty)/6}} e^{i a \tilde{\Delta}_\phi(\infty) k} . \] (5.3a)

\[ C_p(j - k) = \frac{1}{|j - k| \sqrt{K(\infty)/6}} e^{i a \tilde{\Delta}_p(\infty) k} . \] (5.3b)

Hence, \( \tilde{\Delta}_\phi(\infty) \) and \( \tilde{\Delta}_p(\infty) \) are the pitches \( Q_\phi \) and \( Q_p \).

But why should one believe that the two hamiltonians (5.1) and (5.2) are in the same universality class? One reason for this belief is that they have similar duality properties. The hamiltonian (5.1) has a dual symmetry under

\[ \phi_{n+1} - \phi_n \leftrightarrow a p_n ; \]

\[ \Delta_\phi \leftrightarrow \Delta_p ; \]

\[ \gamma_s \leftrightarrow \gamma_v ; \]

\[ \beta \leftrightarrow \beta^{-1} . \] (5.4)
while (5.2) has a similar dual symmetry under

\[ \phi_{n+1} \rightarrow \phi_n + a p_n, \]
\[ \delta_{\phi} \rightarrow \delta_p, \]
\[ \gamma_1 \rightarrow \gamma_2, \]
\[ \beta \rightarrow \beta^{-1}. \]  

Further justification for the Hamiltonian (5.2) comes from the fact that it may be derived from the fermion model \( H_2 = H_1 + W_2 \) of subsect. 4.3. In Appendix B we show that \( H_2 \) is equivalent, in the continuum limit, to

\[
H = \sum_n \frac{1}{2} K \left( \nabla \phi_n \right)^2 + \frac{1}{2} a^2 p_n^2 + a \mu p_n \nabla \phi_n \\
- u_1 \cos \left( 3 \phi_n + 2 \pi n \delta_{\phi} \right) - u_2 \cos \left( 6 \phi_n + 4 \pi n \delta_{\phi} \right) \\
- u_1 \cos \left( 2 \pi \sum_{m=1}^n p_m + 2 \pi n \delta_p \right) - u_2 \cos \left( 4 \pi \sum_{m=1}^n p_m + 4 \pi n \delta_p \right).
\]  

Before discussing how the different terms in (5.6) relate to the ones in \( H_2 \), and how the coupling constants are related to those in \( H_2 \), compare (5.6) with (5.2). Eq. (5.6) can be thought of as having originated from (5.2) after many renormalization transformation steps. The higher harmonics of the two basic vortex and spin wave operators, in addition to the ones shown in eq. (5.6), will be generated during renormalization. In principle, these operators could influence the critical behaviour, but we shall see that they are always irrelevant in the floating phase.

This method of obtaining the continuum formulation of the model has an advantage in that it easily recognizes the excitations which might break up the floating phase. But its weakness is that it cannot tell how the renormalized coupling constants are related to the original ones. The renormalization equations are only known exactly in the limit of small fugacities, while \( \gamma_1 \) and \( \gamma_2 \) are presumed to be large in eq. (5.1). So, it is not certain if indeed there is a floating phase, and, if it exists, it is not clear where it is located. This is why the fermion method of sect. 4 is important; the free fermion model establishes the existence of the floating phase near \( \Delta = \frac{1}{2} \), for small \( \beta \).

In Appendix B we mention the well-known fact that a lattice free fermion model can be converted into a sine-Gordon model like the one obtained from (5.6) after setting \( \mu = u_1 = u_2 = 0 \), with a special fixed value of \( K \), namely \( K = \frac{1}{2} \). This replacement is valid in the scaling limit.

Furthermore, the Hamiltonian \( H_2 \) of subsect. 4.3, which includes all effects of second order in \( \beta \) (or \( 1/\beta \)) leads to the remaining terms in eq. (5.6). The coupling
constants $\mu$, $u_s$, $u_{2s}$ and $u_{2v}$ are small. It is possible, at least in principle, to obtain the renormalized coupling constants in eq. (5.6) as a power series in $\beta$ (or $\beta^{-1}$) and $\frac{1}{2} - \Delta$.

We will now explain where the different operators of eq. (5.6) originate in the continuum limit of the fermion model $H_2 = H_t + W_2$ of sect. 4, and also how their coupling constants behave in lowest order around $\beta = 0, \Delta = \frac{1}{2}$; see eqs. (4.2)–(4.11) and eq. (4.23). For more details see appendix B.

The fugacity $u_s$ is proportional to $\beta$. Its operator is already present in the hopping interaction of the free fermion model (see subsect. 4.2), but not in an explicit way. The role of this operator in the continuum model is to mimic the finite bandwidth, $\beta$, i.e., to produce a finite maximum number of fermions. $u_{2v}$ is proportional to $\beta^2$.

It is the fugacity of the umklapp operator which is hidden in the interactions between fermions, like $\sigma_r \sigma_{r+1}$. The dislocation operator $\sigma_r \sigma_{r+1} \sigma_{r+2}$ gives rise to the continuum operator with a fugacity $u_s = \beta^2$. The continuum operator with fugacity $u_{2s} - \beta^4$ creates (or annihilates) six domain walls. All other higher harmonics of the two basic operators have fugacities which are of successively higher order in $\beta$.

The presence of the stress term $\rho \varphi \phi$ is not obvious from eq. (5.2). In the fermion approach it is generated, because at the Fermi surface the dispersion relation for the hopping terms in $H_2$ implies that the group velocity for a wave packet of left-moving particles is different from that for right-moving ones (see appendix B). The fugacity $\mu$ vanishes at $\Delta = \frac{1}{2}$ as $\mu \sim \beta^2 (\Delta - \frac{1}{2})$.

In the limit $\beta \downarrow 0$ the model reduces to a free fermion model. This implies that the gaussian coupling constant takes the value $K = \frac{3}{8}$. In order $\beta^2$ the fermions attract each other. This implies that $K$ increases when $\beta$ is slightly different from zero as

$$K = \frac{3}{8} + O(\beta^2). \quad (5.7a)$$

The hamiltonian of eq. (5.6) is still self-dual. Indeed, the fermion expansion around $\Delta = \frac{1}{2}, \beta = \infty$ leads to results which are dual to those for small $\beta$. Again the fugacities go to zero: $u_s - \beta^{-1}, u_v - \beta^{-2}, u_{2s} - \beta^{-1}, u_{2v} - \beta^{-4}, \mu - (\frac{1}{2} - \Delta) \beta^{-2}$, but not the gaussian coupling constant, $K$, which decreases with deviations from $\beta = \infty$ as

$$K = \frac{3}{8} - O(\beta^{-2}). \quad (5.7b)$$

Eqs. (5.7a) and (5.7b) give, respectively, the extreme values of $K$ which occur at the lower and upper ends of the $\beta > 0$ incommensurate phase shown in fig. 2. From duality it follows that along $\beta = 1$, $K$ takes the value one. To get additional information, we write the renormalized coupling parameters $K$, $Q_\phi$ and $Q_\rho$ in terms of the original model parameters as

$$K = G(\beta, \Delta_\phi, \Delta_\rho),$$

$$Q_\phi = \Delta_\phi + F_\phi(\beta, \Delta_\phi, \Delta_\rho),$$

$$Q_\rho = \Delta_\rho + F_\rho(\beta, \Delta_\phi, \Delta_\rho). \quad (5.8)$$
Because of the periodic behaviour of the original Hamiltonian in $\Delta_{\theta}$ and $\Delta_{\rho}$, $G$, $F_{\theta}$ and $F_{p}$ are each periodic functions of $\Delta_{\theta}$ and $\Delta_{\rho}$. Under $\Delta_{\theta} \rightarrow -\Delta_{\theta}$, $F_{\theta} \rightarrow -F_{\theta}$ while $G$ and $F_{p}$ remain invariant. Similarly, if $\Delta_{\rho}$ changes sign so does $F_{p}$, but $F_{\theta}$ and $G$ are unchanged.

The dual symmetry implies that if $\beta > 0$,

$$
\left[ G\left(\beta^{-1}, \Delta_{\rho}, \Delta_{\theta}\right) \right]^{-1} = G(\beta, \Delta_{\theta}, \Delta_{\rho}),
$$

$$
F_{p}\left(\beta^{-1}, \Delta_{\rho}, \Delta_{\theta}\right) = F_{\theta}(\beta, \Delta_{\theta}, \Delta_{\rho}).
$$

(5.9)

A kind of initial condition upon $F_{\theta}$ and $F_{p}$ is derived from chiral invariance at $\Delta_{\theta} = 0$, namely

$$
F_{\theta}(\beta, 0, \Delta_{\rho}) = \begin{cases} 
0, & \text{for } \beta > 0, \\
-\frac{1}{\beta}, & \text{for } \beta < 0,
\end{cases}
$$

(5.10)

and correspondingly

$$
F_{p}(\beta, \Delta_{\theta}, 0) = 0.
$$

(5.11)

Then the invariance under $\beta \rightarrow -\beta$ and $\Delta_{\theta} \rightarrow \frac{1}{\beta} - \Delta_{\theta}$ [see eq. (2.7)] becomes

$$
G(\beta, \Delta_{\theta}, \Delta_{\rho}) = G\left(-\beta, \frac{1}{\beta} - \Delta_{\theta}, \Delta_{\rho}\right),
$$

$$
F_{p}(\beta, \Delta_{\theta}, \Delta_{\rho}) = F_{p}\left(-\beta, \frac{1}{\beta} - \Delta_{\theta}, \Delta_{\rho}\right),
$$

$$
F_{\theta}(\beta, \Delta_{\theta}, \Delta_{\rho}) = -F_{\theta}\left(-\beta, \frac{1}{\beta} - \Delta_{\theta}, \Delta_{\rho}\right) - \frac{1}{\beta}.
$$

(5.12)

For $\beta < 0$, the dual symmetry is the statement

$$
\left[ G\left(\beta^{-1}, \frac{1}{\beta} - \Delta_{\rho}, \frac{1}{\beta} - \Delta_{\theta}\right) \right]^{-1} = G(\beta, \Delta_{\theta}, \Delta_{\rho}),
$$

$$
- F_{p}\left(\beta^{-1}, \frac{1}{\beta} - \Delta_{\rho}, \frac{1}{\beta} - \Delta_{\theta}\right) = F_{\theta}(\beta, \Delta_{\theta}, \Delta_{\rho}) - \frac{1}{\beta}.
$$

(5.13)

These results are consistent with the $Q_{\rho}$ assignments for the disordered phases shown in fig. 2, and with the $Q_{\theta}$ assignments for the ordered phases. Of course, in the ordered phase, the renormalized coupling, $G$, is infinite. In the disordered phase it is zero.

Some especially simple results can be obtained from $\Delta_{\theta} = \Delta_{\rho} = \Delta$. Write the corresponding $F$'s and $G$ as $F_{\rho}(\beta, \Delta)$, $F_{\theta}(\beta, \Delta)$ and $G(\beta, \Delta)$.

From eq. (5.9), for $\beta > 0$

$$
G(\beta^{-1}, \Delta) = \left[ G(\beta, \Delta) \right]^{-1},
$$

$$
F_{p}(\beta^{-1}, \Delta) = F_{\theta}(\beta, \Delta).
$$

(5.14)
so that at $\beta = 1$ and $\Delta_0 = \Delta_p$,

$$K = 1, \quad Q_0 = Q_p.$$  \hfill (5.15)

The corresponding statements for $\beta < 0$ are

$$G(\beta^{-1}, \frac{1}{2} - \Delta) = [G(\beta, \Delta)]^{-1},$$

$$F_p(\beta^{-1}, \frac{1}{2} - \Delta) + F_q(\beta, \Delta) = \frac{3}{4}.$$  \hfill (5.16)

These statements enable us to infer the rough shape of contours of equal $K$, $Q_0$ and $Q_p$ shown in figs. 5, 4, and 3 in the introduction.

5.2 STABILITY OF THE FLOATING PHASE FOR $\beta > 0$

We shall now discuss the nature of the transition from the incommensurate floating phase to the ordered and disordered commensurate phases.

The free fermion analysis of sect. 4 showed that, to lowest order in $\beta (1/\beta)$ around $\Delta = \frac{1}{2}$, the transition is Pokrovskii-Talapov-like. We will see that this is likely to remain true for all values of $\beta$. Kosterlitz-Thouless-like melting of the domain walls occurs only at the points $G$, $E$ and $E'$ of fig. 2 (for $\beta < 0$, see subsect. 5.3). In addition, we will show that there are no commensurate "holes" in the floating phase.

It is necessary to test the stability of the massless phase with respect to the spin wave and vortex excitations that are present in the model, eq. (5.6). There are two different mechanisms which determine this stability. First, we should examine the dependence of the vorticity and spin wave number on the coupling constant $K$ of the free scalar field model. The fugacity $u_s$ (or $u_v, u_{2s}, u_{2v}, \ldots$) flows to zero under renormalization if its conjugate operator is irrelevant. To see this, simply calculate the critical exponent, $x$, of the correlation function in the free field theory. If $x > 2$, the operator is irrelevant. From our definition of $K$ and $\mu$ one finds (see ref. [15] or [17])

$$\langle 0 | \cos(\phi_{+} - \phi_{-}) \rangle n(0) - \frac{1}{r^{2x_{s_0}}} \cos(anr\Delta_0),$$  \hfill (5.17)

$$\langle 0 | \cos\left(2\pi m \sum_{i=1}^{s+\tau} p_i \right) \rangle 0) - \frac{1}{r^{2x_{s_0}}} \cos(2\pi mr\Delta_p),$$  \hfill (5.18)

with

$$x_{s, \tau} = \frac{n^2}{6\sqrt{K}} + \frac{1}{2} m^2 \sqrt{K}.$$  \hfill (5.19)

The exponents are independent of $\mu$. 


The exponents vary continuously with $K$; $K$ varies between $\frac{1}{2} < K < \frac{3}{2}$. Only $\cos 3\phi$ and $\cos 2\pi \sum_{m=1}^{n} p_m$ become relevant in this domain. All of their higher harmonics can therefore be neglected in eq. (5.6). There are no commensurate holes in the floating phase.

The second aspect which determines the stability of the massless phase, are the phase factors $2\pi n \Delta$ in the spin wave and vortex operators. Oftlund, in his model, can argue that the floating phase at large $\beta$ will be broken up by a Kosterlitz-Thouless mechanism. The domain wall network melts by unbinding of pairs of dislocations at the value of $\beta$ where the critical exponent $x_{0,1}$ of the operator $\cos(2\pi \sum \rho)$ becomes relevant ($x_{0,1} < 2$). In our model this does not happen because the dislocation operator has a phase factor $2\pi n \Delta_{\rho}$ at $\Delta_{\rho} = \frac{1}{2}$, it becomes exactly staggered:

$$O_{\alpha} = (-1)^n \cos \left(2\pi \sum_{m=1}^{n} p_m \right).$$ (5.20)

In the free scalar field theory a staggered operator does not lead to singularities in the ground-state energy. In the two-dimensional, gaussian language this is usually argued as follows [21]. Calculate the correlation function of this operator by writing it as a "dipole":

$$G = \langle 0 | (O_n - O_{n+1}) (O_{n+r} - O_{n+r+1}) | 0 \rangle$$

$$= \frac{\partial^2}{\partial r^2} \langle 0 | O_n O_{n+r} | 0 \rangle$$

$$\sim \frac{1}{r^{2(x+1)}}.$$ (5.21)

The critical exponent is equal to that of the non-staggered operator, plus one. Actually one can just as well argue that it is equal to $x + 2$, by writing the operator as a "quadrupole", or as $x$ plus any other integer. This ambiguity does not appear in the thermodynamic quantities. The susceptibility $\chi$ is equal to the volume integral (in two dimensions) of the correlation function. By partial integration this is equal to the value of the non-staggered correlation function at the integration boundaries. Therefore, $\chi$ is zero, except for a non-singular short-range contribution, due to the replacement of a discrete derivative by a continuous one in (5.21).

Hence, the dislocations in our model are not able to melt the domain wall network by a Kosterlitz-Thouless mechanism. The floating phase extends at $\Delta_{\rho} = \frac{1}{2}$ all the way down to $\beta = 0$. At $\Delta_{\rho} \neq \frac{1}{2}$ there has to be a phase transition because the model certainly becomes disordered at small $\beta$. The transition is not Kosterlitz-Thouless-
like, but is a standard C-1 phase transition. This can be shown by comparing the results of the fermion expansion about large and small $\beta$ (see subsect. 4). In the $1/\beta$ expansion the operator $\cos(2\pi \Sigma \rho)$ in (5.6) is identified as the dislocation operator $\sigma_n^+ \sigma_n^+ \sigma_{n+2}^- + \text{h.c.}$ which creates and destroys angular domain walls. In contrast, this operator conserves the number of fermions, or momentum domain walls, in the context of the small $\beta$ expansion.

Notice that the $\beta$ and $1/\beta$ expansions use different types of domain walls. The ones for small $\beta$ coincide with the eigenstates of the momentum operator, while the ones at large $\beta$ are identified with the eigenstates of the angle operators $\theta_n$. For small $\beta, \cos 3\theta$ is the dislocation operator while $\cos(2\pi \Sigma \rho)$ conserves the number of domain walls. For large $\beta$ their role is reversed. In the small $\beta$ expansion the operator $\cos(2\pi \Sigma \rho)$ arises from the finite bandwidth of the free fermion model. The lattice fermion model has a cosine-shaped dispersion relation (cf. fig. 13). However, the continuum fermion model has a linear spectrum in eq. (B.14). The operator $\cos(2\pi \Sigma \rho)$ generates gaps in this spectrum precisely at the extrema of the cosine.

The finite bandwidth of the free fermion model confirms that $\cos(2\pi \Sigma \rho)$ has a relevant critical exponent $(x_{0,1} < 2)$ for small $\beta$. However, when the momentum pitch $Q_p$ is far from 0 or $\pm 1$ this gap does not appear at the Fermi surface, and does not lead to the breakup of the floating phase.

In the language of the continuum limit of (5.6) this can also be stated as follows: In the free field theory, both the angular and momentum pitches are conserved quantum numbers. It is convenient to think in terms of the equivalent fermion representation: In the Tomonaga-Luttinger model [cf. eq. (B.14)] there are two types of fermions, right and left movers ($a_R$ and $a_L$), which interact with each other according to a linear dispersion relation. The chemical potentials, $\Delta_p$ and $\Delta_\theta$, change the two Fermi levels. The ground state is defined by a certain number of momentum domain walls (the total number of fermions; conjugate to $\Delta_p$), and angular domain walls (the difference between the number of right and left moving fermions; conjugate to $\Delta_\theta$). Both are good quantum numbers. In our model, however, the operators $\cos(2\pi \Sigma \rho)$ and $\cos(3\theta)$ are included. For small $\beta, \cos(2\pi \Sigma \rho)$ is relevant $(x_{0,1} < 2)$. This operator only conserves $Q_p$. On the other hand, $\cos(3\theta)$ does not conserve $Q_p$, but this operator is irrelevant $(x_{3,0} > 2)$ for small $\beta$. It renormalizes the energy spectrum slightly (by order $\beta^2$), but does not generate a gap. Therefore, at small $\beta$ we can use the momentum domain wall picture. In the same way, the angular domain walls, corresponding to the angular pitch, are, for scaling limit purposes, conserved at large values of $\beta$. From eqs. (5.17)–(5.19) it follows that there is an intermediate temperature interval where both operators are relevant. There, both pitches are not conserved. The relevancy of the operators $\cos(2\pi \Sigma \rho)$ and $\cos(3\theta)$ only affects the eigenstates around integer values of the pitches, $Q_p = 0, \pm 1, \ldots, Q_\theta = 0, \pm 1, \ldots$. Only there do these operators generate gaps in the spectrum of the free field theory, and generate in that way commensurate phases with a finite correlation length, and renormalize the coupling constants significantly.
Along each C-I phase boundary (cf. figs. 2–4), one of the two pitches takes the special value of 0 or ±1. Only at the Lifshitz points do the pitches lock in at the same value, e.g. at point $B, Q_p = Q_o = 0$.

In sect. 4 we showed that the transition into the commensurate phases is second order, Pokrovskii-Talapov-like, in the limit of large and small $\beta$. The nature of this transition probably remains the same for all values of $\beta$ since it is a consequence of the quadratic shape of the dispersion relation in the vicinity of a gap.

A more precise argument can be given as follows: For small $\beta$, only $\cos(2\pi \sum \rho)$ is relevant, and so eq. (5.6) reduces to a sine-Gordon model (after a duality transformation). Recently, Schulz [32] studied the sine-Gordon model with no stress term, i.e. $\mu = 0$. His calculation gives the following general rule: At the C-I phase boundary, the effective coupling constants of the free field theory describing the incommensurate phase take the values for which the critical exponent of the (vortex or spin wave) operator which characterizes the commensurate phase takes the free fermion value, $x = 1$.

This can be understood as follows from the fermion picture. The number of domain walls goes to zero close to the C-I transition. Their mean separation will become much larger than the interaction length, which, in the effective hamiltonian $H_2$ of sect. 4, is only between nearest neighbours. Therefore, we can neglect the interaction terms. Since only hopping terms remain in $H_2$, the model reduces again to a free fermion model, and so the nature of the I-C phase transition is the same as it is in lowest order. The free field coupling constant takes the value $K = \frac{4}{3}$ at the phase boundary (see fig. 5).

This argument goes through in higher order in $\beta$. The assumption that the dislocation operator is irrelevant close to the C-I transition is consistent with the assumption that the number of domain walls goes to zero continuously. But this does not prove that the nature of the C-I transition is the same everywhere, especially around $\beta = 1$ where the high and low temperature C-I lines meet. The transition might become first order. Also, it is not possible to predict the value of $\Delta$ corresponding to the Lifshitz point.

In the floating phase the correlation functions satisfy extended scaling relations which are independent of the coupling constant. For the order and disorder operators

$$O_H = \cos \phi_n, \quad (5.22)$$

$$O_D = \cos \sum_{m=1}^{n} \rho_m, \quad (5.23)$$

these relations are

$$x_H = \frac{1}{3}x_{3,0}, \quad x_{Hx_{0,1}} = \frac{1}{4}. \quad (5.24)$$

$$x_D = \frac{1}{3}x_{0,1}, \quad x_{Dx_{3,0}} = \frac{1}{4},$$

$$x_Dx_H = \frac{1}{36}. \quad (5.24)$$
So at the C-I phase boundary at the $\beta < 1$ ($\beta > 1$) side the exponents take universal values. Because $x_{0,1}$ ($x_{3,0}$) becomes equal to one at the C-I transition, $x_H$ and $x_D$ take the values $x_H = \frac{1}{2}$, $x_D = \frac{1}{2}$ ($x_H = \frac{1}{2}$, $x_D = \frac{1}{2}$). At $\beta = 1$ (for all $\Delta$) $x_H$ and $x_D$ are equal because of duality: $x_H = x_D = \frac{1}{2}$.

5.3. THE PHASE DIAGRAM FOR $\beta < 0$

The phase diagram for negative $\beta$ has two floating phases. Recall that here the phase diagram is invariant under the transformation $\beta \rightarrow \beta^{-1}$, $\Delta \rightarrow \frac{1}{2} - \Delta$. The essential difference from $\beta > 0$ is that in this case the phase factors of the order operators are shifted: $\Delta_\theta \rightarrow \Delta_\theta - \frac{1}{2}$.

In the free fermion approximation this follows from the fact that for $\beta < 0$ the minimum of the dispersion relation is located at $k = \Delta a - \pi$, instead of $k = \Delta a$. For negative values of $\beta$, the single-particle mass gap $m(q)$ (see sect. 3) vanishes first at $q = \Delta - \frac{1}{2}$ (around $\Delta = \frac{1}{2}$). In eq. (5.2) $\Delta_\theta$ is also effectively shifted as $\Delta_\theta \rightarrow \Delta_\theta - \frac{1}{2}$ during the expansion of the cosine in eq. (5.1).

At $\Delta = \frac{1}{2}$ the phase factor of the order operator $\cos(3\phi)$ vanishes. This operator is not staggered now in contrast to the case in which $\beta > 0$. It is now possible for the domain wall network to melt by the Kosterlitz-Thouless mechanism of unbinding of dislocations. This occurs at the value of $K$ where the critical exponent $x_{3,0}$ becomes equal to two. Because we do not know the precise dependence of $K$ on $\beta$, it is not known for which value of $\beta$ this happens. However, because at $\beta = 0$, $x_{3,0} = \frac{3}{2}$ which is already close to 2, it is likely that $|\beta_\Delta| \ll 1$. Locally around $\beta_\Delta$ the model can be described by a sine-Gordon model with a small misfit field proportional to $\Delta - \frac{1}{2}$. Two C-I transition lines will emerge from the isolated Kosterlitz-Thouless point, with an exponential cusp.

The same arguments that we used for $\beta > 0$ show that the effective free field coupling constant $K$ in the incommensurate phase will vary between $\frac{3}{2}$ and $\frac{9}{2}$ (for $\Delta = \frac{1}{2}$). We cannot predict the precise behavior of the C-I transitions in the region around $\Delta = \frac{1}{2}$ where the different C-I transition lines meet.

Appendix A

CONNECTION TO STATISTICAL MECHANICS

According to the usual correspondence rules (see Kogut [2]) one can relate the ground-state properties of a hamiltonian system in one dimension to the statistical mechanical properties of a two-dimensional, but highly anisotropic system. The statistical mechanical system corresponding to the $H$ of eq. (1.5) has a set of variables $\theta_{a,k}$ which take on the values $0, \pm 1$. The partition function takes the form

$$Z = \lim_{T \rightarrow 0^+} \sum_{\{\theta_{a,k} = 0, \pm 1\}} \exp(H_1 + H_2). \quad (A.1)$$
Here, \( H_1 \) corresponds to the second set of terms in eq. (1.5) and is simply

\[
H_1(\theta) = \tau \sum_{j,k} \cos(\theta_{j+1,k} - \theta_{j,k} - \Delta \phi) a. \tag{A.2}
\]

Similarly, \( H_2(\theta) \) describes a set of nearest-neighbour interactions in the "\( k \)" direction and has

\[
H_2(\theta) = \sum_{j,k} t(\theta_{j,k} - \theta_{j,k+1}), \tag{A.3}
\]

\[
e^{i(\theta - \theta')} = \langle \theta | e^{i \cos(\rho - \Delta \phi) a} | \theta' \rangle, \tag{A.4}
\]

which reduces to

\[
t(\theta - \theta') = (\ln \tau/2)(1 - \delta_{\theta,\theta'}) - \frac{\pi^2}{\sqrt{3}} \Delta \phi \sin(\theta - \theta') a, \tag{A.5}
\]

for small \( \tau \).

For \( \Delta \rho = 0 \), the calculation described by eqs. (A.1)–(A.4) is a perfectly standard statistical mechanical problem, with all probabilities positive and all couplings real. However, if \( \Delta \rho \neq 0 \), \( H_2 \) is complex, and the calculation of (A.1) cannot be described in the usual statistical mechanical terms since \( e^{H_1 + H_2} \) is not real, and hence \( (1/Z)e^{H_1 + H_2} \) is not a probability.

This is not a trivial difficulty. The results generated by the partition function calculation of eq. (A.1) are really very different from those of the usual statistical mechanics. To see this point consider the trivial example of a one-dimensional chain described by \( H_1 = 0 \) and thus by a set of variables \( \theta_k, k = 0, 1, 2, \ldots, N \).

The partition function calculation is then given by

\[
Z = \sum_{(\theta_k = 0, \pm 1)} U(\theta_0, \theta_N) \prod_{k=1}^{N} e^{(\theta_k - \theta_{k-1})}. \tag{A.6}
\]

The extra factor \( U(\theta_0, \theta_N) \) is used to represent the boundary conditions at the end of the chain. One can think of several possible cases. A free boundary condition is generated by

\[
U(\theta_0, \theta_N) = U_{\text{free}}(\theta_0, \theta_N) = 1. \tag{A.7a}
\]

A kind of periodic boundary condition is generated by the opposite limit

\[
U(\theta_0, \theta_N) = U_{\text{per}}(\theta_0, \theta_N) = \delta_{\theta_0, \theta_N}. \tag{A.7b}
\]
In general one can most effectively represent \( U(\theta_0, \theta_N) \) by writing it in Fourier series language as

\[
U(\theta_0, \theta_N) = \sum_{p, p' = -1} U(p, p') e^{ip\theta} e^{-i\alpha p\theta_0}.
\]  

(A.8)

Since eq. (A.4) defines the Fourier transform of \( e^{i(\theta - \theta')} \) to be given by

\[
\sum_{\theta'} e^{i(\theta' - \theta')} e^{ip\theta'} = e^{ip\theta} \lambda'(p),
\]

\[
\sum_{\theta} e^{i(\theta - \theta')} e^{-ip\theta} = e^{-ip\theta} \lambda'(p),
\]

(A.9)

with

\[
\lambda(q) = e^{\cos(q - \Delta_p)a}.
\]

(A.10)

The partition function (A.6) reduces to

\[
Z = \sum_{q = -1} U(q, q) [\lambda(q)]^{N\tau}.
\]

(A.11)

Now we see the peculiar feature of the complex terms in \( t(\theta - \theta') \). If \( t(\theta - \theta') \) were real then \( \lambda(q) \) would be largest for \( q = 0 \). This holds, for example, when \( \Delta_p = 0 \) or indeed when \( -\frac{1}{2} < \Delta_p < \frac{1}{2} \). Then, only the term with \( q = 0 \) contributes to the partition function in the limit \( N\tau \rightarrow \infty \) and then, assuming \( \tilde{U}(0, 0) = 0 \),

\[
Z = \tilde{U}(0, 0) \exp\left[ N\tau \cos(a\Delta_p) \right], \quad |\Delta_p| < \frac{1}{2}.
\]

(A.12a)

However, for complex \( t(\theta - \theta') \) it is possible that \( \lambda(1) \) or \( \lambda(-1) \) is larger in magnitude than \( \lambda(0) \). For example if \( \frac{1}{2} < \Delta_p < \frac{3}{2} \), \( \lambda(1) \) is largest, and if \( \tilde{U}(1, 1) \neq 0 \)

\[
Z = \tilde{U}(1, 1) \exp\left[ N\tau \cos(\Delta_p - 1)a \right], \quad \frac{1}{2} < \Delta_p < \frac{3}{2}.
\]

(A.12b)

A comparison of eq. (A.12a) with eq. (A.12b) clearly shows a discontinuity in \( \partial \ln Z / \partial \Delta_p \) at \( \Delta_p = \frac{1}{2} \) and hence a kind of first-order phase transition.

No ordinary statistical mechanical system forming a linear chain ever has such a first order (or any) phase transition. Worse yet, the existence or non-existence of such a phase transition is intimately linked to the exact nature of the boundary condition. For the periodic boundary condition, \( \tilde{U}(q, q) = \frac{1}{2} \) for all \( q \). Hence in this case there is a phase transition. In the free case \( \tilde{U}(q, q) = \delta_{q,0} \). Hence the form (A.12a) holds for all \( \Delta_p \) and there is no phase transition.
Appendix B

In this appendix we derive the continuum limit Hamiltonian of eq. (5.6) from the effective fermion Hamiltonian $H_2 = H_I + W_2$ [see eqs. (4.12) and (4.23)], which represents the original three-state model exactly up to order $\beta^2$. We will use the same method and notation of ref. [15]. This method of obtaining the continuum limit model originates with Luther and Peschel [12]. See also refs. [13, 14].

Apply the Jordan-Wigner transformation [see eq. (4.13)]. In fermion language $H_2$ becomes

$$H_2 = -\sum_x (\mu + (\frac{1}{2}\beta)^2/g) a^+(x)a(x) + \frac{1}{2} \beta (a^+(x)a(x+1)e^{i\alpha} + h.c.)$$

$$+ \left(\frac{(\frac{1}{2}\beta)^2}{g}\right)(a^+(x)a(x+1)e^{-2i\alpha} + h.c.)$$

$$+ \left(\frac{(\frac{1}{2}\beta)^2}{g}\right)(a^+(x+1)a(x+2)e^{2i\alpha} + h.c.)$$

$$+ \left(\frac{(\frac{1}{2}\beta)^2}{g}\right)(a^+(x)a(x)[\frac{1}{2}a^+(x+1)a(x+1) + \frac{1}{2}a^+(x-1)a(x-1)$$

$$- 2(a^+(x+1)a(x-1)e^{-2i\alpha} + h.c.)]$$

$$+ \left(\frac{(\frac{1}{2}\beta)^2}{g}\right)(a^+(x)a^+(x+1)a^+(x+2) + h.c.) \exp i\pi \sum_{y=1}^{x-1} a^+(y)a(y).$$

(B.1)

The extra contribution to the four-fermion interaction comes from the next-nearest-neighbour hopping term.

Consider the free fermion piece of $H_2$, i.e., only the hopping terms and the chemical potential term. Again (see subsect. 4.2) this piece of $H_2$ is diagonal in Fourier language:

$$H_{FF} = \sum_k \left[ \mu - \beta \cos(k - \Delta a) + \left(\frac{1}{2}\beta\right)^2/g - \left(\frac{1}{2}\beta\right)^2/g \right] \cos(k + 2\Delta a)$$

$$- \left(\frac{(1/2)^2}{g}\right) \cos(2k - 2\Delta a) \right] a^+(k)a(k).$$

As before, $\mu$ controls the number of fermions. The second-order contribution to the nearest-neighbour hopping term makes the dispersion relation asymmetric. The band
minimum is no longer at \( k = \Delta a \). Notice that eq. (B.2) gives the single fermion mass gap \( m(q) \) up to order \( \beta^2 \). The four fermion operators need at least two fermions to be effective, while the dislocation operator only gives corrections of order \( \beta^4 \). The value of \( q \) for which \( m(q) \) vanishes for the smallest value of \( \beta \), which determines the C-I phase boundary (see sect. 3), deviates in order \( \beta^2 \) from \( q_c = \Delta \).

Let \( k_F^{(+) and k_F^{(-)} \) be the fermion momenta at the Fermi surface (see fig. 13) and let \( \nu^{(+)} \) and \( -\nu^{(-)} \) be the slope of the dispersion relation at the Fermi surface. First, linearize the dispersion relation at the Fermi surface, and identify the states around \( k_F^{(+)} \) with right moving particles and those around \( k_F^{(-)} \) with left moving ones. Then, translate in momentum space:

\[
a_R(k) = a(k - k_F^{(+)},
\]
\[
a_L(k) = a(k - k_F^{(-)}),
\]

for \( |k| < k_c \); \( \nu \) is the cutoff. In linearized form the free fermion model becomes

\[
H_{FF} = \sum_k \left[ \nu^{(+)} a_R^+(k) a_R(k) - \nu^{(-)} a_L^+(k) a_L(k) \right]
\]
\[
= \sum_x \left[ \nu^{(+)} a_R^+ \frac{\partial}{\partial x} a_R - \nu^{(-)} a_L^+ \frac{\partial}{\partial x} a_L \right].
\]

The formal method of obtaining the continuum limit for the four-fermion interaction and the dislocation operator is to translate them into momentum language and to distinguish all processes which take place at the Fermi surface. A shortcut which avoids some of the paperwork is the replacement of each fermion operator, in real space, by

\[
a(x) \rightarrow a_R(x) e^{ik_F^{(+)}} + a_L(x) e^{ik_F^{(-)}},
\]

and then letting the lattice constant become very small.

There are four different characteristic contributions hidden in the four-fermion terms. They are the same ones as in the XXZ model [12-15].

The contributions with only fermions of one kind, such as

\[
a_R^+(x) a_R(x) a_R^+(x + 1) a_R(x - 1) \exp(-2i\alpha a - 2ik_F^{(+)})
\]

give rise to the continuum operator \( \rho_R^{(x)} \rho_R^{(x)} \). The density operators \( \rho_R \) and \( \rho_L \) are defined so that their expectation value in the free fermion model is zero

\[
\rho_i = a_i^+ a_i - \frac{1}{2} \frac{k_F^{(+) - k_F^{(-)}}}{2\pi}.
\]
Before linearization one should subtract from the chemical potential precisely the amount that is needed to write all the effective density-density operators from the four-fermion interaction in terms of \( \rho_L \) and \( \rho_R \) [24].

As usual, the \( \rho_L \rho_L \) and \( \rho_R \rho_R \) contributions can be absorbed in the slopes \( \nu^{(+)} \) and \( \nu^{(-)} \) of the dispersion relation.

The next characteristic term from the four-fermion interaction,

\[
a_R^-(x)a_L^+(x+1)a_L^-(x-1)\exp(-2ia\Delta - 2ik_{F}^{(-)}),
\]

(B.9)
gives rise to the interaction \( \rho_L \rho_L \) of the Tomonaga-Luttinger model. Also, the backward scattering contributions,

\[
a_R^+(x)a_L^-(x)a_L^+(x+1)a_R^-(x-1)\exp(-2ia\Delta - i(k_{F}^{(+)} + k_{F}^{(-)})),
\]

(B.10)
lead to the Luttinger interaction \( \rho_R \rho_L \).

Finally, there are umklapp operators, such as

\[
a_R^+(x)a_L^-(x)a_R^-(x+1)a_L^+(x-1)\exp(-2ia\Delta - i(k_{F}^{(+)} + k_{F}^{(-)}))
+ 2i(k_{F}^{(-)} - k_{F}^{(+)})x.
\]

(B.11)
They remain composite operators in the continuum fermion model. Only after bosonization do they become point-like objects. The same is true for the dislocation operator. This operator contains two characteristic contributions:

\[
a_R^+(x)a_R^-(x+1)a_L^+(x+2)\exp\left[\frac{i\pi}{x-1} \sum_{y=1}^{x-1} (\rho_R(y) + \rho_L(y))\right]
\times \exp\left[-\frac{1}{2}i(k_{F}^{(+)} + k_{F}^{(-)})(x+1)\right] + \text{h.c.},
\]

(B.12)
\[
a_R^+(x)a_L^+(x+1)a_L^-(x+2)\exp\left[\frac{i\pi}{x-1} \sum_{y=1}^{x-1} \rho_R(y) + \rho_L(y)\right]
\times \exp\left[-i\frac{1}{2}k_{F}^{(+)} + \frac{i}{2}k_{F}^{(-)}\right](x+1)] + \text{h.c.}
\]

(B.13)
So, we end up with a Tomonaga-Luttinger model

\[
H_L = \sum_x iv^{(+)}a_R^+ \frac{\partial}{\partial x} a_R - iv^{(-)}a_L^- \frac{\partial}{\partial x} a_L + \lambda \rho_L \rho_R,
\]

(B.14)
to which are added umklapp and dislocation interactions.
The next step is the bosonization. It is well known that the excitations of the Tomonaga-Luttinger model have a boson character [12]. Therefore the hamiltonian of eq. (B.14) can be rewritten as a free scalar field theory (see e.g., sect. 1 in ref. [15]).

\[ H_L = \sum_x \left( \frac{1}{2} \sigma (v - \lambda) p^2 (x) + \frac{1}{2} \pi (v + \lambda) \left( \frac{\partial \phi}{\partial x} \right)^2 + \mu p (x) \frac{\partial \phi}{\partial x} \right), \quad (B.15) \]

\[ \sigma = \frac{1}{2} (\sigma^+ + \sigma^-), \]

\[ \pi = \frac{1}{2} (\pi^+ - \pi^-). \quad (B.16) \]

The momentum and position operators are defined as

\[ p (x) = \rho_R + \rho_L, \quad (B.17) \]

\[ \frac{\partial \phi}{\partial x} = \pi (\rho_R - \rho_L). \quad (B.18) \]

It is well known that the fermion operators which make up the umklapp and dislocation operators can be replaced by boson operators [12];

\[ a_R (x) \rightarrow \exp \left[ -i \phi (x) - \pi \sum_{\eta = 1}^x p (y) \right], \quad (B.19) \]

\[ a_L (x) \rightarrow \exp \left[ -i \phi (x) + \pi \sum_{\eta = 1}^x p (y) \right]. \quad (B.20) \]

In the boson representation the umklapp operator becomes a vortex operator

\[ y_{2v} \cos \left[ 4 \pi \sum_{y=1}^x p (y) + 2 \pi (k_{p}^+ - k_{p}^-) x \right]. \quad (B.21) \]

The first dislocation operator [eq. (B.12)] becomes a sine-Gordon interaction

\[ y_{4} \cos \left[ 3 \phi (x) + \frac{1}{2} (k_{p}^+ + k_{p}^-) x \right]. \quad (B.22) \]

The second one is a contraction of a sine-Gordon and vortex operator:

\[ y_{sv} \cos \left[ 3 \phi (x) + 2 \pi \sum_{y=1}^x p (y) + \frac{1}{2} (k_{p}^+ + k_{p}^-) x + \left( k_{p}^+ - k_{p}^- \right) x \right]. \quad (B.23) \]

The fugacities \( y_{2v}, y_{4}, y_{sv} \) and the coupling constants \( \lambda, \nu, \mu \) of the free scalar field
part of the Hamiltonian are known in principle to second order in $\beta^2$, but they are rather complicated functions of $\Delta$ and $\beta$. Their gross features, however, such as the fact that $\lambda$, $\nu$, $y_x$, and $y_y$ are proportional to $\beta^2$, are easy to see.

The operator with fugacity $y_x$ is always irrelevant (see sect. 5), so it can be neglected if one is only interested in the structure of the phase diagram. If, however, one wishes to calculate the precise dependence of the critical exponents on $\beta$ and $\Delta$, then it must be realized that this operator renormalizes the coupling constants $\lambda$ and $\nu$. In this renormalization, the higher harmonics such as $\cos 6\phi$, and gradient operators, also become important. They arise from higher order $W_n$ contributions, or from the continuum limit procedure, and also in the continuum model during renormalization.

The only operator which is present in the José et al. derivation of the continuum limit [see eq. (5.6)], but does not appear in the fermion approach is

$$u_x \cos \left[ 2\pi \sum_{y=1}^{x} p(y) + \left( k_F^+ - k_F^- \right) x \right]. \tag{B.24}$$

In the José et al. method this operator mimics the finite bandwidth of the free fermion model. The fermion representation of this operator is a staggered version of the usual mass term of the Thirring model [see eqs. (B.19), (B.20)]:

$$a_R^+(x) a_L^-(x) \exp \left[ \left( k_F^+ - k_F^- \right) x \right] + \text{h.c.} \tag{B.25}$$

This operator generates a gap in the linear dispersion relation of the Luttinger model (with $\lambda = 0$) at precisely the values of $k$ where the dispersion relation of the original free fermion lattice model has its minimum and maximum. Notice that this operator is generated if we apply eq. (B.6) to a hopping operator. We have chosen to put all the effects of the hopping operators into the dependence on $\Delta$ and $\beta$ of the parameters $\nu^+$, $\nu^-$, $k_F^+$ and $k_F^-$. One could set apart a piece of the hopping terms before linearization. This would generate this operator. In the Thirring model one can transform it away again by a Bogolubov transformation.

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