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Two-dimensional Ising model with competing interactions: floating phase, walls and dislocations

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Résumé. — On étudie analytiquement un modèle d'Ising anisotrope bidimensionnel avec interactions en conflit (le modèle « ANNNI » de Selke). On peut en première approximation à basse température décrire le système comme une succession de bandelettes positives et négatives de longueur infinie, séparées par des parois. Dans cette approximation il apparaît trois phases : la phase ferromagnétique, la phase (+ + − − + + − −) et une phase « flottante » avec variation continue du vecteur d'onde. Quand on tient compte des dislocations du réseau des parois, il apparaît en outre une phase paramagnétique. Le domaine de stabilité de cette phase s'étend selon la présente théorie jusqu'à la température nulle. Ceci est en désaccord avec les résultats déduits de simulations sur ordinateur par Fisher et Selke. Le diagramme de phase est très différent de celui du modèle tridimensionnel qui présente une infinité de phases commensurables.

Abstract. — A two-dimensional, anisotropic Ising model with competing interactions (Selke's « ANNNI » model) is studied by analytic methods. As a first approximation the system is described as a sequence of infinite stripes of positive and negative spins separated by « walls ». The phase diagram exhibits three phases : the ferromagnetic phase, a phase with two « up » layers followed by two « down » layers, and so on, and a « floating » phase with continuously varying wave vector. If dislocations of the wall array are taken into account an additional, paramagnetic phase appears. The paramagnetic phase is argued to extend down to zero temperature in disagreement with results deduced from computer simulations by Selke and Fisher. The present results are in strong contrast with those obtained in the corresponding three-dimensional model which exhibits an infinity of locked, commensurate phases.

1. Introduction. — Ising models with competing interactions between nearest neighbours and next nearest neighbours in one direction were first introduced by Elliott [1]. The specific model considered in this paper is displayed by figure 1 in d = 2 dimensions. The interest in this type of model was recently renewed when Bak and Von Boehm [2, 3, 4] investigated the details of the phase diagram numerically and analytically. For d = 3 they found an infinity of commensurate and incommensurate phases. The nature of the commensurate phases at low temperature was specified by Villain and Gordon [5] and by Fisher and Selke [6]. However, the approximations used for d = 3 fail in two dimensions. For d = 2, computer simulations and various approximations have been used by Hornreich et al. [7] and by Selke and Fisher [8]. In this paper a different analytic approach is used in order to specify the nature of the phases. Some of our results are in qualitative disagreement with those of earlier authors.
For \( d = 3 \) all structures obtained at low temperature exhibit conventional order in the average value \( \langle S_i \rangle \) of the spins. At low temperature \( \langle S_i \rangle \) is close to \( +1 \) or \(-1\) for appropriate spin units. Such a structure will be called «pinned». For \( d = 2 \) it will be argued that no pinned structure can be stable except the following three which are known to be stable at \( T = 0 \):

i) the ferromagnetic structure \((++++)\),

ii) the simple antiferromagnetic structure 
\(-++--++--\),

iii) the structure \((+++--++)\) or \((2)\) in the Fisher and Selke [6] notation.

Apart from pinned structures «floating» phases are often encountered in two-dimensional systems. They are characterized by the algebraic decay of spin correlations at long distances \( r, \langle s(0)s(r) \rangle \sim 1/r^\nu \). This possibility of floating phases was first pointed out by Wegner [9] for XY magnets, and by Jancovici [10] for harmonic solids. The transition to the paramagnetic or liquid state (characterized by \( \langle s(0)s(r) \rangle \sim e^{-\alpha r} \)) was investigated by Kosterlitz and Thouless [11] and by Kosterlitz [12], and Nelson and Halperin [13].

The expression «floating phase» was introduced by the latter authors. It has been argued by Bak [14] by mapping the present model onto a Kosterlitz-Thouless model with «cos \( \Phi \) » perturbations [15] that at high temperatures near \( T_c \) a floating phase could exist, in agreement with speculations by Selke and Fisher, but in agreement with predictions made independently of us by Coppersmith et al. [19].

In this paper a rectangular sample of \( N_x \times N_y \) sites is considered. The \( x \) axis is the horizontal direction of figures 1, 2, 3, 4. The \( y \) axis is the vertical axis. The length unit is the interatomic distance. The coordinates \( x, y \) of each sites are integers. Periodic boundary conditions are generally assumed along the \( x \) direction. The temperature \( T = 1/\beta \) is measured in such units that the Boltzmann constant is 1. The energy of a pair of parallel spins is \( J_{0}, J_{1} \) or \( J_{2} \) (Fig. 1). The energy of a pair of antiparallel spins is \( -J_{0}, -J_{1} \) or \( -J_{2} \). These conventions are those of Fisher and Selke [6, 8].

\( J_{0} \) and \( J_{1} \) are assumed to be positive. The value \( J_{1} = J_{0} \) is chosen for all numerical examples.

\[
\begin{align*}
+ &+ -- + + + + + + + + + \\
+ &+ -- + + + + + + + + \\
+ &+ -- + + + + + + + + \\
+ &+ -- + + + + + + + + \\
+ &+ -- + + + + + + + + \\
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+ &+ -- + + + + + + + + \\
+ &+ -- + + + + + + + + \\
+ &+ -- + + + + + + + + \\
+ &+ -- + + + + + + + + \\
\end{align*}
\]

Fig. 2. — A ground state configuration.

2. The free fermion approximation (FFA). — Let the case \( J_{2} = - J_{1} \) be considered first. The ground state is highly degenerate and consists of alternating positive and negative stripes (Fig. 2). Each stripe is bounded by straight «walls» parallel to the \( y \) axis, and its width is \( 2 \) or larger.

In this section we use an approximation [20] in which the excited states also consist of \( v = N_x q \) alternating positive and negative stripes, but the walls are no longer straight. Thus, the width of the \( p \)th stripe depends on the ordinate \( y \). The position \( x_p(y) \) of the \( p \)th wall is assumed to be a single-valued function of \( y \). In analogy with the ground state it is assumed to satisfy the condition (Fig. 3)

\[
x_{p+1}(y) - x_{p}(y) \geq 2 \quad (2.1)
\]
Excited states. The configuration (a) is included in the FFA. The configuration (b) violates condition (2.1) and may be neglected at low temperature. It can probably be neglected at all temperatures of interest without qualitative consequences. Configurations (c) and (d) are neglected in the FFA. Their effect is considered in section 4.

which is reasonable if
\[ T \ll |J_2| \, . \] (2.2)

At low temperatures we may assume
\[ |x_p(y + 1) - x_p(y)| = 0 \text{ or } 1 \] (2.3)

which requires
\[ T \ll J_0 \, . \] (2.4)

The assumption that \( x_p(y) \) is a single-valued function of \( y \) excludes walls which turn back (Fig. 3c, d), as is compatible with condition (2.4). Periodic boundary conditions are assumed in the \( x \) direction:
\[ x_p(y) = x_p(y) + N_x = x_{p + i}(y) \, . \] (2.5)

The problem can be transformed into a standard one by the transformation:
\[ \xi_p(y) = x_p(y) - p \, . \] (2.6)

This transformation depends on the number \( v \) of domains. It can only be performed if \( x_p \) is a uniform function of \( y \). It transforms the system into a system of \((N_x - v) \times N_y\) sites with periodic boundary conditions along \( x \):
\[ \xi_p(y) = \xi_p(y) + N_x - v = \xi_{p + i}(y) \, . \] (2.7)

Periodic boundary conditions will not be assumed along the \( y \) direction. Indeed, even if they are satisfied in the real system (Fig. 4a) they are not conserved in the transformed system (Fig. 4b).

Variables \( \xi_p \) satisfy the following relations:
\[ |\xi_{p + i}(y) - \xi_p(y)| \geq 1 \] (2.8)
\[ |\xi_p(y + 1) - \xi_p(y)| = 0 \text{ or } 1 \, . \] (2.9)

The partition function is then given by
\[ Z(v) = \sum \langle 1 | \hat{\theta} | 2 \rangle \langle 2 | \hat{\theta} | 3 \rangle \ldots \langle N_y - 1 | \hat{\theta} | N_y \rangle \times \exp - 2 \beta v(J_1 - 2 | J_2 \rangle N_y \] (2.10)

where \( |y\rangle \) denotes the set \{ \( \xi_1(y), \xi_2(y), \ldots, \xi(v) \) \}, and the summation is over all possible sets \{ \( \xi_p(y) \) \}. The transfer matrix \( \hat{\theta} \) is defined as follows:
\[ \langle y | \hat{\theta} | y + 1 \rangle = 0 \text{ if } \xi_p(y) \text{ and } \xi_p(y + 1) \]
do not satisfy conditions (2.7), (2.8), (2.9). If these conditions are satisfied
\[ \langle y | \hat{\theta} | y \rangle = 1 \, , \]
\[ \langle y | \hat{\theta} | y + 1 \rangle = \exp - 2 \beta m J_0 \]

when \( \xi_p(y + 1) - \xi_p(y) = 0 \) for \( (v - m) \) values of \( p \) while the other \( m \) values satisfy
\[ \xi_p(y + 1) - \xi_p(y) = \pm 1 \, . \]

The set \( |y\rangle \) may be associated with a state with \( v \) fermions at \( \xi_p(y) \):
\[ |y\rangle = c^+(\xi_1(y)) c^+(\xi_2(y)) \ldots c^+(\xi(v)) |\text{vac}\rangle \, . \] (2.11)

where \( |\text{vac}\rangle \) is the state with zero fermions. The transfer matrix then takes the form
\[ \theta = 1 + \gamma \sum_{\xi} \left[ c^+ (\xi) c (\xi + 1) + c^+ (\xi + 1) c (\xi) \right] + \gamma^2 \sum_{\xi \neq \xi'} \left[ c^+ (\xi) c (\xi + 1) + c^+ (\xi + 1) c (\xi) \right] \times \left[ c^+ (\xi') c (\xi' + 1) + c^+ (\xi' + 1) c (\xi') \right] + \cdots \]  

(2.12)

where

\[ \gamma = \exp(-2\beta J_0). \]  

(2.13)

Equation (2.12) does not reproduce those matrix elements for which \( \xi_{x+1}(y + 1) = \xi_y(y) \). However, this error is small if condition (2.4) is satisfied. Making similar approximations on the omitted terms, the transfer matrix (2.12) can be written as the exponential of a free fermion Hamiltonian, namely

\[ \theta = \exp \gamma \sum_{\xi} \left[ c^+ (\xi) c (\xi + 1) + c^+ (\xi + 1) c (\xi) \right]. \]  

(2.14)

Now, let \( |0\rangle \) be the eigenvector of \( \theta \) corresponding to the largest eigenvalue \( E_0 \). Formula (2.10) reads:

\[ Z(v) = E_0^{N_x} \exp \left[ -2\beta v N_x (J_1 + 2J_2) \right] \sum_{(\xi \in \{1\})} \sum_{(\xi' \in \{N_y\})} \langle 1|0\rangle \langle 0|N_x, N_y \rangle \]

\[ = E_0^{N_x} \exp \left[ -2\beta v N_x (J_1 + 2J_2) \right] C(v). \]  

(2.15)

The factor

\[ C(v) = E_0^{-1} \sum \langle 1|0\rangle \langle 0|N_x \rangle \]  

(2.16)

reflects the influence of the upper and lower boundaries, and its dependence on \( v \) vanishes in the thermodynamic limit \( N_x, N_y \to \infty \).

For the sake of simplicity, we shall now assume periodic boundary conditions instead of (2.5) and the transfer matrix can be written

\[ \theta = \exp(-\mathcal{K}) \]  

(2.17)

where

\[ \mathcal{K} = -\gamma \sum_{\xi} \left[ c^+ (\xi) c (\xi + 1) + c^+ (\xi + 1) c (\xi) \right] \]

\[ = -2\gamma \sum_{k} c_k^+ c_k \cos k, \]  

(2.18)

and \( c_k \) is the Fourier transform of \( c(\xi) \).

The lowest eigenvalue of \( \mathcal{K} \) is clearly obtained for

\[ |0\rangle = \prod_{-k_F < k < k_F} c_k^+ \mid \text{vac} \rangle \]  

(2.19)

where

\[ k_F = \pi v (N_x - v) \]  

(2.20)

and \( k \) is any integer multiple of \( 2\pi/(N_x - v) \) satisfying the condition \( -\pi < k < \pi \). The largest eigenvalue of \( \theta \) is

\[ E_0(v) = \exp 2\gamma \sum_{k=-k_F}^{k_F} \cos k \]

\[ = \exp \left[ \frac{2\gamma}{\pi} (N_x - v) \int_0^{\pi} \cos k \, dk \right]. \]  

(2.21)

\[ = \exp \left[ \frac{2\gamma}{\pi} (N_x - v) \sin \frac{\pi v}{N_x - v} \right]. \]  

(2.22)

Dropping the factor \( C(v) \), equations (2.15) and (2.21) yield:

\[ Z = \exp N_x \left[ -\frac{2\gamma}{\pi} (N_x - v) \sin \frac{\pi v}{N_x - v} - 2\beta v (J_1 + 2J_2) \right]. \]  

(2.23)

The number of walls, \( v \), is obtained by maximizing (2.22). The density of walls

\[ q = v/N_x \]  

is given, using formula (2.13), by

\[ \frac{1}{1 - q} \cos \frac{\pi q}{1 - q} - \frac{1}{\pi} \sin \frac{\pi q}{1 - q} = \beta (J_1 + 2J_2) \exp(2\beta J_0). \]  

(2.24)

This equation has a non-trivial solution (i.e., neither \( q = 0 \) nor \( q = 1/2 \)) if

\[ -2T \exp(-2\beta J_0) < J_1 + 2J_2 < T \exp(-2\beta J_0). \]  

(2.25)

Above this interval the system is ferromagnetic (\( q = v = 0 \)) and below this interval \( q = \frac{1}{2} \). Inside the interval (2.24) the « wave vector » \( q \) giving the periodicity of the structure varies continuously with \( J_2/J_1 \), in contrast with the 3d behaviour. The phase transition lines given by (2.24) are shown in figure 5, and the wave vector as a function of \( (J_1 + 2J_2) \) is shown in figure 6.

The phase boundary of the ferromagnetic state can be calculated following the method of Müller-Hartmann and Zittarz [21] which gives [7, 22].

\[ \sinh \left[ 2\beta (J_1 + 2J_2) \right] \sinh 2\beta J_0 = 1. \]  

(2.26)
Fig. 5. — Phase diagram for $J_1 = J_2 > 0$. Full lines are derived from (2.24) in the low temperature region and from (2.25) for $J_2 \approx 0$. The dashed line is plotted using (4.3) and (4.5). F = ferromagnetic phase. P = paramagnetic phase. FL = floating phase.

Fig. 6. — Wave vector as a function of $x = -(J_1 + 2J_2)/T$ in the floating phase.

In the low temperature limit (2.4), equation (2.25) becomes

$$\beta(J_1 + 2J_2) = \exp(-2\beta J_0)$$

in agreement with (2.24).

3. Fluctuations and correlations in the FFA in the floating phase. — Let point $(x, y)$ lie in the $n$'th stripe. The field $n(x, y)$ is related to the spin $S_n(x, y)$ at site $(x, y)$ by the relation:

$$S_n(x, y) = \exp i \pi n(x, y).$$

The average value of $n$ is

$$\overline{n(x, y)} = qx$$

and its fluctuation is

$$\frac{1}{\pi} \varphi(x, y) = n(x, y) - qx.$$

Correlation functions are more easily evaluated in the fictitious system $(\Sigma)$ deduced from the real system $(S)$ by the transformation (2.6). More precisely this transformation associates to the point $(x, y)$ of $(S)$ the point $(\zeta, y)$ of $(\Sigma)$ defined by:

$$\zeta = x - n(x, y).$$

If the point $(x, y)$ of the real system lies in the $n$'th stripe, the point $(\zeta, y)$ of the fictitious system lies in the $n$'th stripe in view of formulae (2.6) and (3.4). It is therefore natural to define in $(\Sigma)$ the field:

$$\overline{n(\zeta, y)} = n(x, y)$$

where $\zeta$ and $x$ are related by (3.4). The average value of $\overline{n}$ is:

$$\overline{n(\zeta, y)} = \frac{q}{1-q} \zeta$$

and its fluctuation is

$$\frac{1}{\pi} \varphi(\zeta, y) = \overline{n(\zeta, y)} - \frac{q}{1-q} \zeta.$$

Replacing $\overline{n}$ and $\zeta$ by their expressions (3.5) and (3.4) and using (3.3), one obtains:

$$\overline{\varphi(\zeta, y)} = \frac{1}{1-q} \varphi(x, y).$$

The calculation of correlation functions in the fictitious system $(\Sigma)$ is a well-known problem [23, 20]. It is performed in Appendix A for both directions $x$ and $y$. Both results are consistent with formula:

$$\left< [\varphi(\rho' + \rho) - \varphi(\rho')]^2 \right> = \left[ 1 + \left( \frac{1}{\rho} \right) \ln \rho \right].$$

It may be argued that this formula holds for any vector $p = (\zeta, y)$ of $(\Sigma)$. Formula (3.9) is consistent with a Landau-Wilson free energy of the form

$$F = \frac{1}{2} \int d\zeta \, dy \left[ \overline{K_\zeta} \left( \frac{\partial \varphi}{\partial \zeta} \right)^2 + \overline{K_y} \left( \frac{\partial \varphi}{\partial y} \right)^2 \right]$$

or

$$F = \frac{1}{2} \int dX \, dY \sqrt{\overline{K_\zeta}} \overline{K_y} \left[ \left( \frac{\partial \varphi}{\partial X} \right)^2 + \left( \frac{\partial \varphi}{\partial Y} \right)^2 \right]$$

where:

$$\overline{K_\zeta} = \zeta(\overline{K_\zeta}/\overline{K_y})^{1/4}, \quad \overline{K_y} = y(\overline{K_\zeta}/\overline{K_y})^{1/4}$$

and

$$\sqrt{\overline{K_\zeta}} \overline{K_y} = T/\pi.$$

The derivation of (3.9) from (3.11) and (3.13) is straightforward [9]. Formulae (3.11) and (3.13) will therefore be accepted without further proof. It can probably be derived from renormalization group theory as done by Knops [24] in a related but somewhat different problem.

The next step of the argument is to come back to the real system $(S)$. The relation with $(\Sigma)$ is provided by relation (3.4) which can be differentiated as follows:

$$d\zeta = dx - \left( \frac{dn}{dx} \right) dx - \left( \frac{dn}{dy} \right) dy$$
or, using (3.3) :
\[ d\zeta' = \left(1 - q - \frac{1}{\pi} \frac{\partial \phi}{\partial \xi} \right) dx - \frac{1}{\pi} \frac{\partial \phi}{\partial \eta} dy. \quad (3.14) \]

On the other hand, relation (3.8) can be differentiated as follows :
\[
\left( \frac{\partial \phi}{\partial \xi} \right) d\zeta' + \left( \frac{\partial \phi}{\partial \eta} \right) dy = \frac{1}{1 - q} \left( \frac{\partial \phi}{\partial \xi} \right) dx + \frac{1}{1 - q} \left( \frac{\partial \phi}{\partial \eta} \right) dy.
\]

Insertion of expression (3.14) for \( d\zeta' \) yields :
\[
\left[ (1 - q - \frac{1}{\pi} \frac{\partial \phi}{\partial \xi}) \frac{\partial \phi}{\partial \xi} - \frac{1}{\pi} \frac{\partial \phi}{\partial \eta} \right] dx + \left[ \frac{\partial \phi}{\partial \eta} - \frac{1}{\pi} \frac{\partial \phi}{\partial \xi} \right] dy = 0.
\]

Factors multiplying \( dx \) and \( dy \) may be both identified to zero separately. Furthermore we have in mind a long wavelength approximation, so that \( V\phi \) (or \( V\phi \)) may be assumed to be small. The following simple relations are thus obtained :
\[
\frac{\partial \phi}{\partial \xi} = \frac{1}{(1 - q)^2} \frac{\partial \phi}{\partial \xi} \quad (3.15a)
\]
\[
\frac{\partial \phi}{\partial \eta} = \frac{1}{1 - q} \left( \frac{\partial \phi}{\partial \eta} \right)_x. \quad (3.15b)
\]

Insertion into (3.10) yields :
\[
F = \frac{1}{2} \int d\zeta dy \left( \frac{K_x}{(1 - q)^4} \left( \frac{\partial \phi}{\partial \xi} \right)^2 + \frac{K_y}{(1 - q)^2} \left( \frac{\partial \phi}{\partial \eta} \right)^2 \right). \quad (3.16)
\]

In this expression, \( d\zeta' \) may be replaced by \((1 - q) \) \( dx \) which is the approximate form of (3.14). One obtains :
\[
F = \frac{1}{2} \int dx dy \left[ K_x \left( \frac{\partial \phi}{\partial \xi} \right)^2 + K_y \left( \frac{\partial \phi}{\partial \eta} \right)^2 \right]. \quad (3.16)
\]

with
\[
K_x = \frac{K_x}{(1 - q)^4}, \quad K_y = \frac{K_y}{(1 - q)}. \quad (3.17)
\]

Relations (3.13) and (3.17) yield :
\[
\sqrt{K_x K_y} = \frac{T}{\pi(1 - q)^3}. \quad (3.18)
\]

Introducing the new coordinates :
\[
X = x(K_x/K_y)^{1/4}, \quad Y = y(K_x/K_y)^{1/4} \quad (3.19)
\]
the free energy (3.16) takes the more symmetric form :
\[
F = \frac{1}{2} \int dX dY K_x K_y \left[ \left( \frac{\partial \phi}{\partial X} \right)^2 + \left( \frac{\partial \phi}{\partial Y} \right)^2 \right]. \quad (3.20)
\]
\[
= \frac{1}{2} \sqrt{K_x K_y} \sum_k \phi_{-k} \phi_k \quad (3.21)
\]
where \( \phi_k \) is the Fourier transform of \( \phi(x, y) = \phi(r) \).

The mean square fluctuation is readily deduced :
\[
\langle |\phi_k|^2 \rangle = \frac{T}{k^2 \sqrt{K_x K_y}}. \quad (3.22)
\]

The mean square fluctuation in real space :
\[
\langle [\phi(r' + r) - \phi(r')]^2 \rangle = \frac{1}{4\pi^2} \int 2 d^2 k \langle |\phi_k|^2 \rangle (1 - \cos kr)
\]
can be approximated for large \( r \) by
\[
\langle [\phi(r' + r) - \phi(r')]^2 \rangle \approx \frac{T}{\pi \sqrt{K_x K_y}} \ln r. \quad (3.22)
\]

This well known calculation [9] is of course the same which leads from (3.10) to (3.9). The spin pair correlation function can be deduced from (3.1) and (3.3) :
\[
\langle S_x(r' + r) S_x(r') \rangle = \langle \exp im(\phi(r' + r) - \phi(r)) \rangle.
\]

In agreement with (3.16), the random variable \([n(r' + r) - n(r')]\) may be assumed to have a Gaussian probability centred at \( q \). In this case it can be shown (using the fact that \( n \) is an integer) that
\[
\langle \exp[in(n(r' + r) - n(r))] \rangle = \exp \left\{ -\frac{\pi^2}{2} \langle [n(r' + r) - n(r) - q]^2 \rangle \right\} \cos q \xi.
\]

When \( q = 0 \), this relation is well-known [9]. Using (3.22) and (3.18) one finally finds
\[
\langle S_x(r' + r) S_x(r') \rangle \approx r^{-1} \cos q \xi, \quad (3.23)
\]
where
\[
\tau = \frac{1}{2} (1 - q^2). \quad (3.24)
\]

The algebraic decay (3.23) is the signature of two-dimensional « floating » phases [13, 9-12, 20]. It is remarkable that the exponent (3.24) does not depend explicitly on temperature. In particular for \( J_2 = -J_1/2 \), the solution of equation (2.23) is (when \( J, J_0 \))
\[
q = 0.3008 \quad (3.25)
\]
and relation (3.24) yields \( \tau = 0.24 \). This value is independent of \( T \). However it is only correct at low temperature since it is derived from the FFA.

The free energy (3.16) will be used in the next section. For most of the arguments it is sufficient to know the product \( K_x K_y \) given by formula (3.18). However, the separate values of \( K_x \) and \( K_y \) are calculated for the sake of completeness in Appendix B.

4. Dislocations of the wall network. — As argued in the Introduction, the main source of error in the FFA is that walls are not allowed to come backward as shown on figure 7. In the present section this possibility is introduced. The definition of the field \( n(x, y) \)
will first be generalized. It is sufficient to define the variation of \( n(x, y) \) along two kinds of paths:

i) \( n(x, y) \) is a constant integer along any path which does not intersect any wall.

ii) \( n(x, y) \) changes by 1 along a horizontal path going from the left to the right when intersecting a wall, and only in this case. The change is by \(-1\) if one goes from the right to the left.

If walls are not allowed to come backward, \( n(x, y) \) reduces to the single-valued function defined in section 3, except for an additive constant.

Around a closed path encircling the end of a positive or negative domain in the trigonometric sense (Fig. 7) the total change of \( n \) is 2 if the domain comes from the bottom of the sample, and \(-2\) if the domain comes from the top. The field \( \phi(x, y) \) defined by (3.3) changes by \( \pm 2\pi \):

\[
\int \! d\phi = \pm 2\pi. \tag{4.1}
\]

Thus, the wall loops shown in figure 7 can be considered as dislocations of the wall network. Away from dislocations the free energy is given by formula (3.16). Formulae (4.1) and (3.16) constitute the whole basis of the Kosterlitz-Thouless theory. Therefore their presence in the theory of the ANNNI model is sufficient to guarantee the equivalence of this model (in the floating phase) with the XY ferromagnet. In particular, the floating phase is stable with respect to paramagnetism if the following condition is satisfied.

\[
\pi J/T - 1 \geq 2\pi \exp(-\mu/T). \tag{4.2}
\]

This condition corresponds to relations (A.18) and (3.5) of reference [12]. Comparison of formula (2.2) of the same reference with our formula (3.20) shows that \( J \) is to be identified with \( \frac{1}{2}\sqrt{K_x K_y} \). Replacing this quantity by its expression (3.18), condition (4.2) becomes:

\[
\frac{1}{2(1 - q^2)} - 1 \geq 2\pi \exp(-\mu/T). \tag{4.3}
\]

This condition involves the quantity \( \mu \) which is the free energy of an isolated dislocation. The exact definition of \( \mu \) will be found in reference [12]. Condition (4.3) implies the following, weaker condition, which has the advantage to be independent of \( \mu : 2(1 - q^2) < 1 \), or

\[
q > 1 - \frac{1}{\sqrt{2}}. \tag{4.4}
\]

Thus, if \( q \) is calculated from formula (2.23), there is a region near the ferromagnetic part of the phase diagram, where condition (4.4) is not satisfied and therefore the system is paramagnetic (Fig. 5). There is no direct commensurate-incommensurate transition from ferromagnetism to the floating phase. The Lifshitz point is at \( T = 0 \).

For the right hand side of the phase diagram \( (J_1 + 2J_2 < 0) \) it is necessary to know the free energy \( \mu \) of a dislocation. At low temperature \( \mu \) may be replaced by the minimum energy \( 4J_0 \) of a dislocation (see Fig. 7a). At higher temperature, more complex dislocation structures (Fig. 7b) should be taken into account, and one obtains for \( J_1 + 2J_2 \approx 0 \)

\[
\exp(-\beta\mu) = \exp(-4\beta J_0) [1 + 2\exp(-2\beta J_1) + 2\exp(-4\beta J_1) + \ldots]
= \exp(-4\beta J_0) \frac{1 + \exp(-2\beta J_1)}{1 - \exp(-2\beta J_1)}. \tag{4.5}
\]

Figure 5 was plotted using formulae (4.5), (4.3), (2.23) for the paramagnetic-floating transition, and formula (2.24) for the other transitions. The evaluation (4.5) might be refined and this would modify the right hand part of the phase diagram. However we prefer to focus the discussion on more qualitative and more fundamental points.

DISCUSSION. — Our approximate treatment by-passes certain technical complications which would
appear in a complete renormalization group (RG) treatment of the ANNNI model. The normal RG treatment \cite{12, 15} consists in the progressive elimination of dislocation pairs of radius $R < \tau$, where $\tau$ goes from the atomic distance to infinity, and

$$R = \sqrt{X^2 + Y^2} \quad (4.6)$$

$X$ and $Y$ are defined by (3.19). The usual technique assumes \cite{12, 15} a Landau-Wilson free energy of the form (3.20) or (3.31). In the ANNNI problem, this form is only correct for short wave vectors $k \leq R_0$, where $R_0$ is evaluated below, equation (4.8). Longer wave vectors yield a finite energy contribution which has not the form (3.31). Only for $\tau \gtrsim R_0$ the renormalization group equations take the form obtained by Kosterlitz \cite{12} and José \emph{et al.} \cite{15} which only involve two parameters $J = \frac{1}{2}K_x K_y$ and $\mu$.

The description of short wavelength fluctuations would involve more parameters because of the anisotropy. Their elimination by RG would produce, for $\tau \gtrsim R_0$, a two-parameter model, and equation (4.3) would follow. This step (elimination of short wavelengths) has been by-passed in our treatment. A drawback of this simplification is that $\mu$, which is related to dislocation core effects, is not known. However the most spectacular prediction of our theory is the paramagnetic phase extending down to $T = 0$, and this was derived from condition (4.4) which does not depend on $\mu$. On the other hand the evaluation of $J = \frac{1}{2}K_x K_y$ is rather safe since it is related to properties of the system between two dislocations. The only approximation is to assume that these properties are the same as those of an infinite, dislocation-free medium. This looks reasonable, at least at low temperature when the average distance $R_1$ between two dislocations is much larger than $R_0$. In fact, $R_1$ is given by $qR_0^2 \exp(-4 \beta J_0) \approx 1$. $q$ is the probability of having a wall passing at a given point and $\exp(-4 \beta J_0)$ is the probability of having a dislocation at a point of a wall. Therefore

$$R_1 \approx q^{-1/2} \exp(2 \beta J_0). \quad (4.7)$$

A more careful treatment shows that this relation holds only for $q \gtrsim \exp(- \beta J_0)$. The case of smaller $q$, when neighbouring dislocations lie on the same wall, will not be considered here.

$R_0$ is defined by the following two conditions deduced from (3.19).

i) $x_0 = R_0(K_x/K_y)^{1/4}$ is larger than 1/q.

ii) $y_0 = R_0(K_y/K_x)^{1/4}$ is larger than the average distance between two collisions of a wall with the wall at its left and the wall at its right.

Using formulae (B.6) and (B.16), it turns out that both conditions (i) and (ii) yield the same result

$$R_0 \approx q^{-3/2} \exp(\beta J_0). \quad (4.8)$$

Thus $R_0 \ll R_1$ at low temperature if $q \gtrsim \exp(- \beta J_0)$. However formulae (4.7) and (4.8) do not hold when $q$ is very close to 1/2. This case will not be considered here since our treatment seems to agree with numerical simulations \cite{8}.

Even for long wavelengths it is not quite true that the theory contains only two parameters $\mu$ and

$$J = \frac{1}{2}K_x K_y.$$ $q$ is also a parameter. In this paper it was assumed to be constant throughout the RG procedure, and given by the FFA evaluation (2.23). This evaluation looks reasonable at low temperatures.

5. Conclusion. — We have presented an analytic treatment of the two-dimensional ANNNI model. The right hand part ($J_1 + 2J_2 < 0$) of the phase diagram (Fig. 5) is in qualitative agreement with computer simulations \cite{8} but quantitative results rely upon a very rough evaluation of the parameter $\mu$ of formula (4.2).

The left hand part ($J_1 + 2J_2 > 0$) is in severe disagreement with the phase diagram published by Selke and Fisher \cite{8}. A recent work by Coppersmith \emph{et al.} \cite{19} is in agreement with our predictions, and in fact uses the same argument as we use in section 4. The paper by Coppersmith \emph{et al.} is a more general qualitative discussion of commensurate-incommensurate (C-I) transitions in two dimensions, while the present paper is a more detailed and more precise investigation of a special model.

Jaubert \emph{et al.} \cite{25} have recently observed by low energy electron diffraction a C-I transition of a xenon monolayer on the (110) face of copper. The system has an Ising symmetry and the result seems to contradict ours, as well as it is in contradiction with Coppersmith \emph{et al.} However there is no real contradiction at low temperature. Indeed the paramagnetic phase described in section 4 has strongly oscillating correlation functions. The right hand side of (3.22) is multiplied by a damping factor $\exp(- \kappa' x - \kappa'' y)$, but $\kappa'$ and $\kappa''$ are very small at low temperature. The resulting broadening of the Bragg peaks may well be masked by the instrumental resolution. Of course, the experimental system of interest is not an ANNNI model since the interactions decay exponentially with distance \cite{20}. The phase diagram may therefore be quite different, but the existence or non-existence of a C-I transition does not depend on the interaction range, provided it is not infinite.

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**Appendix A.** — The calculation of correlations in the fictitious system (\( \Sigma \)) is a well-known problem [23], the solution of which will be recalled here for completeness. The quantity \( n(x, y) \) defined in section 3 is related to Fermion operators of section 2 by the relation

\[
n(x, y) = n(0, y) + \sum_{\xi_1}^{x - 1/2} \langle y | c^+(\xi) c(\xi) | y \rangle.
\]  

(A.1)

In this Appendix the notations \( n, x \) and \( \varphi \) are used instead of \( \bar{n}, \xi \) and \( \varphi \). There is no confusion because all calculations are done in (\( \Sigma \)) and the real system (\( S \)) does not appear in this Appendix.

Correlations in the \( x \) directions are given in the notations of section 2 by

\[
\langle [n(x', y) - n(x, y)]^2 \rangle = \left\langle 0 \left| \sum_{\xi_1}^{\infty} c^+(\xi) c(\xi) \right| 0 \right\rangle = \left\langle 0 \left| c^+(\xi) c(\xi) \right| 0 \right\rangle = \left\langle n(x', y) - n(x, y) \right\rangle^2 + \frac{1}{(N_x - y)^2} \sum_{k,k' \in \Sigma} \left\langle 0 | c_k^+ c_k c_{k'}^+ c_k | 0 \right\rangle e^{-|k-k'|^2}
\]

or, with

\[
\varphi(x, y) = \pi n(x, y) - \langle n(x, y) \rangle,
\]

\[
\langle [\varphi(x', y) - \varphi(x, y)]^2 \rangle = \frac{\pi^2}{(N_x - y)^2} \sum_{|k| > k_F} \left| 1 - \exp \left( ik \right) \right|^2 = \frac{1}{4} \int_{-k_F}^{k_F} dk' \int_{|k| > k_F} \frac{\sin^2 \left[ (k - k') (x - x') / 2 \right]}{\sin^2 \left( (k - k') / 2 \right)}.
\]

For \( |x - x'| \gg 1 \) the contribution for \( k \approx k' \approx \pm k_F \) is divergent and dominates

\[
\langle [\varphi(x', y) - \varphi(x, y)]^2 \rangle \approx \int_{|k| > k_F} dk' \int_{k_F}^{k_F} dk \frac{1 - \cos (k - k') (x - x')}{(k - k')^2} \approx \int q \frac{1 - \cos q(x - x')}{q^2} \approx \int \frac{1}{1 + |k' - x|} \frac{dq}{q} \approx \ln \left[ |x' - x| \right]. \]  

(A.2)

Correlations in the \( y \) direction can also be deduced from (A.1) provided non-periodic boundary conditions are chosen, so that \( n(x, y) = 0 \) on the left hand edge of the sample. In this case the quantity to be calculated is

\[
G(y) = \langle [n(x, y') + n(x, y)]^2 \rangle = 2 \sum_{k} \left[ 1 - (E / E_0)^2 \right] \left\langle 0 \left| \sum_{\xi_1}^{\xi} c^+(\xi) c(\xi) \right| E \right\rangle^2 \]  

(A.3)

where \( E \) and \( |E| \) are the eigenvalues and eigenvectors of the transfer operator (2.17). It is convenient to assume integer values of \( \xi = -l, -(l - 1), ..., -1, 0, 1, ..., l \) and half integer values of \( x \) ranging from \( - (l + 1/2) \) to \( + (l + 1/2) \). Here \( l + 1 = N_x / 2 \). The fictitious Hamiltonian (2.18) is diagonalized by the following Fourier transform appropriate for non-periodic boundary conditions

\[
c^+(\xi) = (l + 1)^{-1/2} \sum \left( a_k^* \cos k \xi + b_k^* \sin k \xi \right)
\]

(A.4)

with \( k = p \pi / (2 l + 2) \), \( p = 1, 2, 3, ..., 2 l + 1 \).

\( a_k = 0 \) if \( p \) is even, \( b_k = 0 \) if \( k \) is odd.

The vector \( |0\rangle \) is given by formula (2.19) except that \( k \) runs from 0 to \( k_F = \pi q / (1 - q) \). The calculation of (A.3) is lengthy and will only be summarized below. (A.3) may be written as

\[
G(y) = G_1 + G_2 + G_3 + G_4
\]  

(A.5)
where

\[ G_1 = \frac{1}{2} (l + 1)^{-2} \sum \sum [1 - (E/E_0)^2] \langle 0 | a_k^+ a_{k'} | E \rangle \langle E | a_k^+ a_{k'} | 0 \rangle \left[ f\left(\frac{k - k'}{2}\right) + f\left(\frac{k + k'}{2}\right) \right] \quad (A.6) \]

where \( f \) is given for large \( x \) by

\[ f(K) = \cos^2 K(l - x + \frac{1}{2}) \sin^2 K(l + x + \frac{1}{2}) \sin^2 K. \quad (A.7) \]

\( G_2, G_3 \) and \( G_4 \) are deduced from (A.6) by replacing \( a_k \) by \( b_k \) or \( a_k \) by \( b_k \) or both, and by replacing function (A.7) by other appropriate functions.

For given \( k, k' \), the only contribution to (A.6) comes from

\[ | E \rangle = a_k^+ a_{k'} | 0 \rangle \]

so that relations (2.17) and (2.18) yield:

\[ (E/E_0)^p = \exp[-2 \gamma y(\cos k - \cos k')]. \quad (A.8) \]

The sum (A.6) is dominated by the divergence of \( f\left(\frac{k - k'}{2}\right) \) for \( k \approx k' \approx k_F = \pi q/(1 - q) \). Neglecting nondivergent terms, relations (A.5) to (A.8) yield after some calculation

\[ G(y) = \frac{1}{4} (l + 1)^{-2} \sum \sum \frac{1 - \exp[-2 \gamma y(k' - k) \sin k_F]}{(k - k')^2} \]

or, after some additional calculation:

\[ \langle [n(x, y^* + y) - n(x, y^* - y)]^2 \rangle \approx \frac{1}{\pi^2} \ln \left[ \frac{4 \gamma y \pi q(1 - 2 q) \sin \frac{\pi q}{1 - q}}{1 - q} \right] \]

in agreement with (3.9).

**Appendix B.** In this Appendix we calculate the coefficients \( K_x \) and \( K_y \), which appear in the FFA free energy (3.16)

\[ F_0 = \frac{1}{2} \int \int dx \, dy [K_x(\partial_x \varphi)^2 + K_y(\partial_y \varphi)^2] \quad (B.1) \]

where \( \varphi \) is defined by (3.3):

\[ \varphi(x, y) = \pi[n(x, y) - q_0 x] \quad (B.2) \]

and \( q_0 \) is given by (2.23):

\[ \frac{\partial F_0}{\partial q_0}(q_0) = \mathcal{N} \frac{\partial}{\partial q_0} \left[ \frac{2 \gamma T}{\pi} (1 - q) \sin \frac{\pi}{1 - q} + 2 q(J_1 + 2 J_2) \right]_{q=q_0} = 0 \quad (B.3) \]

with \( \gamma = \exp - 2 J_0/T \). We wish to calculate the linear response:

\[ \langle \partial \varphi / \partial x \rangle = \frac{h_x}{K_x} \quad (B.4) \]

produced by an additional free energy term:

\[ \delta F_x = - h_x \int \int dx \, dy \partial \varphi / \partial x \quad (B.5) \]

where \( x = x \) or \( y \). For \( x = x \), (B.5) may be written as:

\[ \delta F_x = - h_x \pi \mathcal{N}(q - q_0). \]
The total free energy is therefore:
\[ F_0 + \delta F_x \approx F_0(q_0) + \frac{1}{2} (q - q_0)^2 \frac{\partial^2 F_0}{\partial q^2}(q_0) - h_x \pi(q - q_0) N. \]

The linear response (B.4) is readily obtained:
\[ \frac{h_x}{K_x} = \left\langle \frac{\partial \varphi}{\partial x} \right\rangle = \pi(q - q_0) = \pi^2 h_x N \left\{ \frac{\partial^2 F_0}{\partial q^2}(q_0) \right\} \]
or, differentiating (B.3):
\[ K_x = \frac{2 T}{\pi(1 - q)^3} \sin \frac{\pi q}{1 - q} \exp - 2 \beta J_0. \] (B.6)

The calculation of \( K_x \) is a little more difficult. The linear response (B.4) has to be calculated from the Hamiltonian:
\[ \mathcal{H} = -\frac{1}{2} \sum_{i,j} J_{ij} S_i^x S_j^z - \delta \mathcal{H}_\nu \] (B.7)

where
\[ \delta \mathcal{H}_\nu = - \pi h_x \sum_{x,y} [n(x, y + 1) - n(x, y)] = - \pi h_x \sum_{x,y} \sigma(x, y). \] (B.8)

The linear response is:
\[ \left\langle \frac{\partial \phi}{\partial y} \right\rangle = \pi \left\langle \sigma(x, y) \right\rangle = \frac{T}{N} \frac{\partial}{\partial h_y} \ln Z \] (B.9)

where the partition function:
\[ Z = \text{Tr} \exp - \beta \mathcal{H} \]
can be calculated by the transfer matrix method as in section 2
\[ Z = N q \exp - 2 \beta(J_1 + 2J_2) \sum_{x,y} E^{y,x-1} \left\langle \alpha \right| E \left\langle \gamma \right. \] (B.10)

where \( \alpha \) and \( \gamma \) are the eigenvectors of \( c^+(\xi) \) \( c(\xi) \), i.e. states with walls at well-defined positions. \( E \) and \( \left\langle E \right. \) designate the eigenvalues and eigenvectors of the transfer matrix:
\[ \tilde{\theta} = \exp - \tilde{\mathcal{H}} \] (B.11)

where, at low temperature:
\[ \tilde{\mathcal{H}} = - \gamma \sum_{\xi} [c^+(\xi) c(\xi + 1) \exp \pi \beta h_y + c^+(\xi + 1) c(\xi) \exp - \pi \beta h_y] = \]
\[ = - \gamma \sum_{k} [\exp(ik + \pi \beta h_y) + \exp -(ik + \pi \beta h_y)] c_k^+ c_k. \] (B.12)

The eigenvectors of this non-hermitian « Hamiltonian » are:
\[ \prod_{k \in \mathcal{K}} c_k^+ \left\langle \text{vac} \right. \]
where \( \mathcal{K} \) designates any subset of the Brillouin zone. The eigenvalues of \( \tilde{\theta} \) are:
\[ E(\mathcal{K}) = \prod_{k \in \mathcal{K}} \exp[\gamma \exp(ik + \pi \beta h_y) + \gamma \exp -(ik + \pi \beta h_y)]. \]

The modulus of this product is less than, or equal to the product of the moduli of its factors
\[ |E(\mathcal{K})| \leq \exp \left[ 2 \gamma (\cosh \beta \pi h_y) \sum_{k \in \mathcal{K}} \cos k \right]. \]
Therefore, for any given number v of walls:

\[ |E(K)| \leq E_0(v) \]

where \( E_0 \) is the real eigenvalue corresponding to the eigenvector (2.19), namely:

\[ E_0 = \exp \left( 2 \gamma \sum_{k=0}^{\infty} \cosh \beta \pi h_y \cos k \right). \]

(B.13)

For large \( N' \) the sum (B.10) is dominated by \( E_0 \). Neglecting other eigenvalues one finds:

\[ Z = C(v) E_0^{N'v} \exp \left( -2 \beta \nu(J_1 + 2 J_2) \right) \]

(B.14)

where \( C(v) \) is defined by (2.16) and may be dropped in the thermodynamic limit. Relations (B.9) and (B.14) yield:

\[
\frac{\partial \varphi}{\partial y} = \frac{T}{N_x} \frac{\partial}{\partial y} \ln E_0
\]

or, according to (B.13):

\[
\langle \frac{\partial \varphi}{\partial y} \rangle = 4 \pi \gamma N_x^{-1} \sum_{k=0}^{\infty} \sinh \beta \pi h_y \cos k = 2 \gamma (1 - q) \sinh \beta \pi h_y \int_0^{\infty} \cos k \, dk
\]

\[ = 2(1 - q) \gamma \sinh \beta \pi h_y \sin \frac{n \pi}{1 - q}. \]

(B.15)

For \( h_y \ll T \), relation (B.4) yields:

\[ K_y = \frac{T \exp 2 \beta \nu_0}{2 \pi (1 - q) \sin \frac{n \pi}{1 - q}}. \]

(B.16)

Formulae (B.6) and (B.16) are in agreement with equation (3.18) which was obtained by a different argument.

References