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## THEORY OF ONE- AND TWO-DIMENSIONAL MAGNETS WITH AN EASY MAGNETIZATION PLANE

### II. THE PLANAR, CLASSICAL, TWO-DIMENSIONAL MAGNET

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**Résumé.** — On donne une nouvelle méthode d'étude des systèmes planaires magnétiques à 2 dimensions : le Hamiltonien est remplacé par une approximation qui, contrairement aux approximations antérieures, préserve la symétrie correcte du problème. On confirme l'existence d'une transition à  $T_c$  et on donne une évaluation quantitative de  $T_c$  et de la fonction de corrélation de paire au-dessous de  $T_c$ . Les résultats sont en accord à basse température avec ceux de l'approximation de Hartree. On prévoit une transition à une température  $K_B T_c = 1,7 J s^2$ , en bon accord avec les prédictions des développements en séries à haute température, alors que les exposants critiques sont ceux prévus par Kosterlitz, notamment  $\gamma = \infty$ .

**Abstract.** — A new approach to the 2-D classical planar magnet is proposed. The Hamiltonian is replaced by an approximate one, which, in contrast with previous approximations, preserves the correct symmetry of the problem ; the existence of a phase transition without long range order at some temperature  $T_c$  is confirmed ; quantitative evaluations of the spin pair correlation function below  $T_c$ , and of the transition temperature  $T_c$  are given ; the results are in good agreement at low  $T$  with the self consistent harmonic approximation (S.C.H.A.). A transition is predicted at a temperature  $K_B T_c = 1.7 J s^2$ , in very good agreement with predictions based on series expansions, whereas the critical exponents are those predicted by Kosterlitz, in particular  $\gamma = \infty$ .

1. **Introduction.** — It is commonly admitted that two-dimensional (2-D) magnets without lattice anisotropy undergo a transition without long range order (L.R.O.) [1, 2] at a finite temperature  $T_c$ , and that L.R.O. appears below  $T_c$  in the presence of the slightest anisotropy or of the slightest three-dimensional (3-D) interactions [3, 4, 5]. In practice, both anisotropy and 3-D interactions are present, so that what is experimentally seen [6, 7] is a critical temperature  $T_c$  (with L.R.O.) which has the same order of magnitude as the in-plane coupling constant  $J$  and is independent of the 3-D interaction  $J' \ll J$ , and of the anisotropy ; this is somewhat unexpected, since L.R.O. should disappear at any finite temperature  $T$  when  $J'$  and the anisotropy vanish [8], so that one might expect  $T_c$  to vanish with  $J'$  and the anisotropy.

Berezinskii and Blank [5] have been able to show that it is actually not so : in the Heisenberg, 2-D model, L.R.O. persists up to a finite temperature, even for vanishingly small  $J'$  or anisotropy. In our point of view, this is the only non-heuristic theory of the 2-D Heisenberg model, although Greens Function

decoupling approximations [2, 3, 4] are apparently in good agreement with experiment. In particular, no reliable description of the transition in the isotropic case exists ; the very existence of the transition has even been questioned [9].

The situation is better in the case of *planar*, classical systems, in which the spin is a 2-D classical vector [10, 11, 12, 13, 14] ; such a model is a poor approximation of any existing material, but it can be expected to have a behaviour quite similar to the Heisenberg model. Most of existing theories [10, 11, 12, 13, 14] are low temperature approximations, and the problem is to extend them to higher temperatures. A fruitful method for this purpose has been developed by Kosterlitz and Thouless [15, 16], who have argued that a 2-D planar classical magnet is equivalent to a 2-D classical electrolyte. By means of this trick, they have been able to give a qualitative description of the region below  $T_c$ , and Kosterlitz [16] was able to give the values of the critical exponents — which are quite unusual, since  $\alpha = -\infty$  and  $\gamma = +\infty$ .

A weakness of the Kosterlitz-Thouless model [15] is that the equivalence between the 2-D planar magnet

and the 2-*D* electrolyte lies on intuitive and qualitative, rather than quantitative bases; this equivalence, rather clear at low *T*, is not at all obvious in the critical region.

In contrast with the Kosterlitz-Thouless approach, qualitatively correct but quantitatively incorrect, another method, the self-consistent harmonic approximation (S.C.H.A.) of Pokrovskii and Uimin [17] is quantitatively correct at low *T* (as will be shown in this paper), but requires better justification, because it replaces the original potential by a potential of a different symmetry, so that it is not obvious that the qualitative features of the model are preserved; moreover, S.C.H.A. is the first step of a perturbation expansion, whose convergence is questionable [14] because fourth order terms in the potential are negative.

The approach proposed in the present paper unifies the methods of Kosterlitz and Thouless, and of Pokrovskii and Uimin, and provides them with better bases. In addition, further improvement of the method can be envisaged.

The approximation proposed in the present paper replaces the magnetic Hamiltonian by an approximate one, which has the complete symmetry of the original Hamiltonian, and which naturally splits into 2 parts : i) a harmonic Hamiltonian,  $\mathcal{H}_h$ , with a *T*-dependent stiffness constant, which exhibits no phase transition, but accounts for the properties of the system up to 0.9  $T_c$ ; the stiffness constant can be expanded in powers of *T*, and the first 2 terms have the same value as in S.C.H.A. ii) a Hamiltonian  $\mathcal{H}_v$ , which describes a 2-*D* electrolyte, with a *T*-dependent Coulomb interaction. The equivalence with the 2-*D* electrolyte is quantitative at all temperatures.

For more generality, an in-plane anisotropy is inserted in the general formalism, but only the properties of the isotropic planar magnet will be described in this paper; the effect of an in-plane anisotropy will be treated in a subsequent paper.

The approach proposed in this paper cannot be easily generalized to 2-*D* quantum magnets, but it can be applied to quantum linear chains, which will be the object of a subsequent article.

The present paper is the continuation of a previous one, mentioned as reference [14].

**2. The model.** — The model, as defined by other authors [10, 11, 12, 15] is described by a continuous, classical field  $\varphi_i$  defined at the sites *i* of a 2-*D* or 3-*D* lattice and representing the polar angle of a 2-*D* unit vector. The energy has the form :

$$\mathcal{H} = \sum_{ij} V_{ij}(\varphi_i - \varphi_j) + \sum_i U(\varphi_i) \quad (2.1)$$

where  $V_{ij}$  is a short range interaction; more precisely, nearest neighbour interactions will be assumed in

the greatest part of this work. Usually, one takes :

$$V_{ij}(\varphi) = -J_{ij} \cos \varphi \quad (2.2)$$

$$U(\varphi) = -D \cos m\varphi \quad (2.3)$$

where  $J_{ij}$  and *D* are constants and *m* is a given integer.  $m = 1$  corresponds to a magnetic field,  $m = 2$ ,  $m = 4$  and  $m = 6$  define an *m*-fold anisotropy; other values of *m* are in principle non-physical.

Instead of (2.2) and (2.3), the following forms of  $V_{ij}$  and *U* will be assumed :

$$V_{ij}(\varphi) = \frac{1}{2} K_B T \text{Log} \sum_{n=-\infty}^{\infty} \exp - \beta A_{ij}(\varphi - 2\pi n)^2 + \text{const.} \quad (2.4)$$

$$U(\varphi) = K_B T \text{Log} \sum_{v=-\infty}^{\infty} \exp - \beta B(\varphi - 2\pi v/m)^2 + \text{const.} \quad (2.5)$$

where *n* and *v* are integers; if (2.4) and (2.5) are used to approximate (2.2) and (2.3), the constants depend on the temperature *T* and are of importance for the calculation of the specific heat but not for the correlation functions. In the calculation of the partition function, correlation functions, etc.,  $V_{ij}$  and *U* appear through the Gibbs distribution, and therefore through the expressions :

$$\exp - 2\beta V_{ij}(\varphi) = \text{const.} \sum_{n=-\infty}^{\infty} \exp - \beta A_{ij}(\varphi - 2\pi n)^2 \quad (2.6)$$

$$\exp - \beta U(\varphi) = \text{const.} \sum_{v=-\infty}^{\infty} \exp - \beta B(\varphi - 2\pi v/m)^2. \quad (2.7)$$

The factor 2 in (2.6) accounts for double summation over each pair.

It results that the correlation functions which can be calculated from (2.4) and (2.5) are exactly those which might be calculated from the following effective Hamiltonian :

$$\hat{\mathcal{H}} = \frac{1}{2} \sum_{ij} A_{ij}(\varphi_i - \varphi_j - 2\pi n_{ij})^2 + B \sum_i \left( \varphi_i - 2\pi \frac{v_i}{m} \right)^2 \quad (2.8)$$

where the  $n_{ij}$ 's satisfy :  $n_{ij} = -n_{ji}$ .

The system is now described by the continuous field  $\varphi_i$  plus the discrete fields  $n_{ij}$  and  $v_i$ . The advantage of this description is that (2.8) is a quadratic form, although non-trivial because of the discrete fields.  $n_{ij}$  and  $v_i$  have no obvious physical meaning.

Real systems are often well described by (2.2) and (2.3), so that expressions (2.4) and (2.5) must be considered as approximate forms in which the parameters  $A_{ij}$  and *B* must be defined as functions

of  $J_{ij}$  and  $K$ . This definition can be provided by the prescription that the right hand sides of (2.6) and (2.7) have the correct first 2 Fourier components, i.e., the first 2 Fourier components must be the same as those of the left hand sides after insertion of (2.2) and (2.3). With such a prescription, the fit is very good at low and high temperature, and satisfactory at intermediate  $T$ , as shown by figure 1, which compares (2.2) and (2.4) near  $T_c$ .

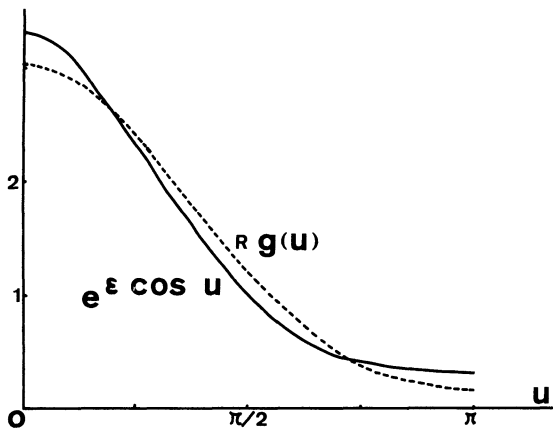


FIG. 1. — The true Boltzmann factor (full line)  $\exp - 2 \beta V$ , where  $V$  is given by (2.2) and the approximate Boltzmann factor resulting from (2.4) (dotted line).

The calculation is given in the appendix. One finds

i) In the high temperature limit :

$$A_{ij} = K_B T / (4 \text{Log } K_B T / J_{ij}) \quad (2.9)$$

$$B = m^2 K_B T / (4 \text{Log } 2 K_B T / D) . \quad (2.10)$$

ii) In the low temperature region :

$$A_{ij} = J_{ij} (1 - K_B T / 4 J_{ij}) . \quad (2.11)$$

Figure 2 gives  $A/J$  as a function of  $T/J$  from 0 to the transition temperature, about  $\pi J / K_B$  [15].

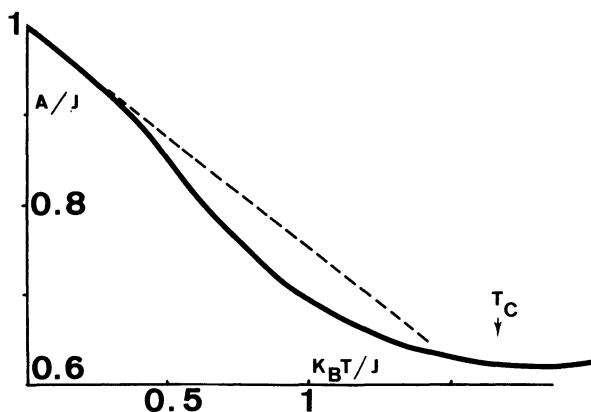


FIG. 2. — Reduced, renormalized stiffness constant  $A/J$  as a function of temperature between 0 and  $T_c$ .

If all  $n_{ij}$ 's are supposed to vanish, and if the first order term in (2.11) is neglected, the Wegner-Berezinskii [10, 11] approximation is recovered at low  $T$ .

We are not yet in a position to take full advantage of the quadratic character of (2.8), because in the expression of the average value of any quantity  $\mathcal{A}$  :

$$\langle \mathcal{A} \rangle = Z^{-1} \text{Tr}^{(n)} \text{Tr}^{(v)} \text{Tr}^{(\varphi)} e^{-\beta \mathcal{H}} \mathcal{A} \quad (2.12)$$

appears an integration over  $\varphi_i$  from  $-\pi$  to  $+\pi$  since :

$$\text{Tr}^{(\varphi)} = \prod_i \int_{-\pi}^{\pi} d\varphi_i \quad (2.13)$$

$$\text{Tr}^{(n)} = \prod_{i < j} \sum_{n_i = -\infty}^{\infty}, \quad \text{Tr}^{(v)} = \prod_i \sum_{v_i = -\infty}^{\infty} . \quad (2.14)$$

It is clearly more convenient to use an integration over  $\varphi_i$  from  $-\infty$  to  $+\infty$ ; this can be achieved by the use of the following identity :

$$\int_{-\pi}^{\pi} d\varphi = \lim_{\varepsilon \rightarrow 0} 2 \sqrt{\beta \pi \varepsilon} \int_{-\infty}^{\infty} d\varphi e^{-\beta \varepsilon \varphi^2} \quad (2.15)$$

where both sides are operators acting on any periodic function of  $\varphi$  at their right, with period  $2\pi$ . Eq. (2.15) can be easily derived from eq. (2.12). Inserting (2.15) and (2.8) into (2.12), it is seen that the average values can be calculated from the Hamiltonian :

$$\hat{\mathcal{H}} = \frac{1}{2} \sum_{ij} A_{ij} (\varphi_i - \varphi_j - 2\pi n_{ij})^2 + B \sum_i (\varphi_i - 2v_i/m)^2 + \varepsilon \sum_i \varphi_i^2 \quad (2.16)$$

using the rules (2.12), (11.14) and :

$$\text{Tr}^{(\varphi)} = \prod_i \int_{-\infty}^{\infty} d\varphi_i \quad (2.17)$$

instead of (2.13).

(2.16) involves a double summation on each pair  $(i, j)$  with  $n_{ij} = -n_{ji}$ . The limit  $\varepsilon \rightarrow 0$  has to be taken.

**MORE SOPHISTICATED APPROXIMATIONS.** — It is possible to have correct first 3 Fourier components, if (2.4) is replaced by the following, more sophisticated expression :

$$V(\varphi) = \frac{1}{2} K_B T \text{Log} \sum_{n=-\infty}^{\infty} \sum_{S^z=-1}^1 \exp - \beta A (\varphi - 2\pi n - \pi - \alpha S^z)^2 \quad (2.18)$$

where  $\alpha$  is a  $T$ -dependent parameter, and  $S^z$  is a spin 1. The reader will easily invent more complicated forms yielding more Fourier components; the approximation (2.18) will be discussed in Chapter 6.

**3. Transformation of the effective hamiltonian in the case of first neighbour interactions.** — Assuming a (2-*D*) rectangular or (3-*D*) orthorhombic lattice with first neighbour interactions, we shall now transform the effective Hamiltonian (2.8). As it is quadratic, a Fourier transformation is relevant :

$$\varphi_k = \frac{1}{\sqrt{N}} \sum_i \varphi_i e^{i\mathbf{k}\cdot\mathbf{R}_i} \quad (3.1a)$$

$$v_k = \frac{1}{\sqrt{N}} \sum_i v_i e^{i\mathbf{k}\cdot\mathbf{R}_i} \quad (3.1b)$$

$$n_k^\alpha = \frac{1}{\sqrt{N}} \sum_{i<j} n_{ij}^\alpha \exp\left(i\mathbf{k}\cdot\frac{\mathbf{R}_i + \mathbf{R}_j}{2}\right) \quad (3.1c)$$

*N* is the number of sites,  $\mathbf{R}_i$  is the vector of the coordinates of the site *i* and  $n_{ij}^\alpha = n_{ij}$  for any bond *ij* directed along  $O\alpha$  ( $\alpha = x, y, z$ ).  $n_{ij}^\alpha = 0$  otherwise.

The non-vanishing possible values of  $A_{ij}$  are called  $A_x, A_y, A_z$ . The effective Hamiltonian (2.16) can be written as :

$$\hat{\mathcal{H}} = \sum_k \left[ \sum_\alpha A_\alpha |iK_\alpha \varphi_k - 2\pi n_k^\alpha|^2 + B \left| \varphi_k - \frac{2\pi}{m} v_k \right|^2 + \varepsilon |\varphi_k|^2 \right] \quad (3.2)$$

where

$$K_\alpha = 2 \sin \mathbf{k}\cdot\mathbf{a}_\alpha/2 \quad (3.3)$$

where  $\mathbf{a}_x, \mathbf{a}_y, \mathbf{a}_z$  are the vectors defining the unit cell.

The summation in (3.2) and in the following is over the Brillouin zone. (3.2) can be cast into the following form :

$$\hat{\mathcal{H}} = \mathcal{H}_h + \mathcal{H}_v + \mathcal{H}_a \quad (3.4)$$

with

$$\mathcal{H}_h = \sum_k \left( B + \sum_\alpha A_\alpha K_\alpha^2 + \varepsilon \right) \theta_k^* \theta_k \quad (3.5)$$

$$\mathcal{H}_v = 4\pi^2 \sum_{kxy} n_{kx} n_{ky}^* \left( A_\alpha \delta_{xy} - \frac{A_\alpha A_\gamma K_\alpha K_\gamma}{\varepsilon + \sum_\xi A_\xi K_\xi^2} \right) \quad (3.6)$$

$$\mathcal{H}_a = \sum_k \frac{B \sum_\alpha A_\alpha K_\alpha^2}{B + \sum_\alpha A_\alpha K_\alpha^2 + \varepsilon} \xi_k^* \xi_k \quad (3.7)$$

where :

$$\xi_k = 2\pi \left( \frac{v_k}{m} + i \frac{\sum_\alpha A_\alpha K_\alpha n_{k\alpha}}{\varepsilon + \sum_\alpha A_\alpha K_\alpha^2} \right) \quad (3.8)$$

and

$$\theta_k = \varphi_k - 2\pi \frac{B \frac{v_k}{m} - i \sum_\alpha A_\alpha K_\alpha n_{k\alpha}}{\varepsilon + B + \sum_\alpha A_\alpha K_\alpha^2} \quad (3.9)$$

or :

$$\varphi_k = \theta_k + \frac{B \xi_k}{B + \sum_\alpha A_\alpha K_\alpha^2 + \varepsilon} - 2\pi i \frac{\sum_\alpha A_\alpha K_\alpha n_{k\alpha}}{\varepsilon + \sum_\alpha A_\alpha K_\alpha^2} \quad (3.10)$$

The variables  $\theta_i$  are continuous and can take all values from  $-\infty$  to  $+\infty$ , so that the harmonic Hamiltonian  $\mathcal{H}_h$  is trivial and contains no phase transitions. It is decoupled from  $\mathcal{H}_v$  and  $\mathcal{H}_a$ .

**4. Vortices.** — 4.1 INTRODUCTION OF THE VORTEX VARIABLES. — In this Section, the relation with the vortices, introduced by Kosterlitz and Thouless [15] will be shown in the special case of 2-*D* systems. Eq. (13.6) reads for  $D = 2$  :

$$\mathcal{H}_v = 4\pi^2 A_x A_y \sum_k \frac{|K_y n_{kx} - K_x n_{ky}|^2}{\varepsilon + \sum_\alpha A_\alpha K_\alpha^2} + 4\pi^2 \varepsilon \sum_k \frac{\sum_\alpha A_\alpha |n_{k\alpha}|^2}{\varepsilon + \sum_\alpha A_\alpha K_\alpha^2} \quad (4.1)$$

In the limit  $\varepsilon = 0$ ,  $\mathcal{H}_v$  does not depend on the variables

$$p_k = i(K_y n_k^x + K_x n_k^y) \quad (4.2)$$

but only depends on the variables :

$$q_k = i(K_y n_k^x - K_x n_k^y) \quad (4.3)$$

It is important to note that the Fourier transforms  $p_\rho$  and  $q_\rho$  are integers. They are defined at the centres  $\rho$  of the unit cells, as follows :

$$p_\rho^x = n_x \left( \mathbf{R}_\rho - \frac{\mathbf{a} + \mathbf{b}}{2}, \mathbf{R}_\rho + \frac{\mathbf{a} - \mathbf{b}}{2} \right) - n_x \left( \mathbf{R}_\rho + \frac{\mathbf{b} - \mathbf{a}}{2}, \mathbf{R}_\rho + \frac{\mathbf{a} + \mathbf{b}}{2} \right) \quad (4.4)$$

$$p_\rho^y = n_y \left( \mathbf{R}_\rho - \frac{\mathbf{a} + \mathbf{b}}{2}, \mathbf{R}_\rho + \frac{\mathbf{b} - \mathbf{a}}{2} \right) - n_y \left( \mathbf{R}_\rho + \frac{\mathbf{a} - \mathbf{b}}{2}, \mathbf{R}_\rho + \frac{\mathbf{a} + \mathbf{b}}{2} \right)$$

$\mathbf{a}$  and  $\mathbf{b}$  are the vectors  $\mathbf{a}_x$  and  $\mathbf{a}_y$  which define the unit cell.

$$p_\rho = p_\rho^x + p_\rho^y = N^{-1/2} \sum_k p_k e^{i\mathbf{k}\cdot\mathbf{R}_\rho} \quad (4.5)$$

$$q_\rho = p_\rho^x - p_\rho^y = N^{-1/2} \sum_k q_k e^{i\mathbf{k}\cdot\mathbf{R}_\rho} \quad (4.6)$$

Insertion of (4.3) into (4.1) yields : in the limit  $\varepsilon = 0$  :

$$\mathcal{H}_v = 4\pi^2 A_x A_y \sum_{k \neq 0} \frac{q_{-k} q_k}{\sum_\alpha A_\alpha K_\alpha^2} \quad (4.7)$$

The term  $k = 0$  has been omitted because

$$q_{k=0} = p_{k=0} = 0 \quad (4.8)$$

as results from the definition (4.4) if cyclic boundary conditions are imposed.

The integers  $q_\rho$  are the charges introduced by Kosterlitz and Thouless.

From now on, one assumes :

$$A_x = A_y = A \quad (4.9)$$

#### 4.2 VORTEX INTERACTION IN THE DIRECT SPACE. —

Because the  $q_\rho$ 's, and not the  $q_k$ 's are integers, it is convenient to rewrite (4.7) in the direct space as :

$$\mathcal{H}_v = \sum_{\rho\rho'} \tilde{V}_{\rho\rho'} q_\rho q_{\rho'} \quad (4.10)$$

where

$$\tilde{V}_{\rho\rho'} = \frac{4\pi^2 A}{N} \sum_{k \neq 0} \frac{e^{ik \cdot (\mathbf{R}_\rho - \mathbf{R}_{\rho'})}}{K_x^2 + K_y^2}$$

can be rewritten as :

$$\tilde{V}_{\rho\rho'} = V_0 + V_{\rho\rho'}$$

where

$$V_0 = \tilde{V}_{\rho\rho} = \frac{4\pi^2 A}{N} \sum_{k \neq 0} \frac{1}{K_x^2 + K_y^2} \simeq 2A \int_{2\pi/L}^{\pi/a} \frac{a^2 d^2k}{K_x^2 + K_y^2}$$

goes to infinity when the dimension  $L$  goes to infinity. This is of no importance, because (4.10) reads :

$$\mathcal{H}_v = \sum_{\rho\rho'} V_{\rho\rho'} q_\rho q_{\rho'} + V_0 \left( \sum_\rho q_\rho \right)^2$$

and the second term vanishes because of the condition (4.8). Finally :

$$\mathcal{H}_v = \sum_{\rho\rho'} V_{\rho\rho'} q_\rho q_{\rho'} \quad (4.11)$$

where

$$V_{\rho\rho'} = -\frac{4\pi^2 A}{N} \sum_k \frac{1 - \cos \mathbf{k} \cdot (\mathbf{R}_\rho - \mathbf{R}_{\rho'})}{K^2 + K_y^2} \quad (4.12)$$

is found to have the following special values :

$$V_{\rho\rho} = 0 \quad (4.13a),$$

$$V_{\rho\rho'} = -\pi^2 A \text{ for nearest neighbours} \quad (4.13b).$$

When the distance  $r_{\rho\rho'}$  between  $\rho$  and  $\rho'$  is large, the asymptotic form of  $V_{\rho\rho'}$  has been given by other authors [11, 16], but a more explicit calculation will be given below;  $V_{\rho\rho'}$  is easily seen to be isotropic for large distances, so that  $\mathbf{r}_{\rho\rho'}$  can be assumed to be parallel to  $Ox$ ; in this case the integration over  $k_y$  can be carried out and yields :

$$-V_{\rho\rho'} = \pi A \int_0^\pi du \frac{1 - \cos nu}{\sin u/2} + \pi A \int_0^\pi du \frac{1 - \cos nu}{\sin u/2} \frac{1 - \sqrt{1 + \sin^2 u/2}}{\sqrt{1 + \sin^2 u/2}}$$

where  $u = k_x a$  and  $\mathbf{r}_{\rho\rho'} = n\mathbf{a}$ ; for large  $n$ , one obtains

$$-V_{\rho\rho'} \simeq 2\pi A \sum_{p=0}^{n-1} \frac{1}{p + \frac{1}{2}} + \pi A \int_0^\pi \frac{du}{\sin u/2} \frac{1 - \sqrt{1 + \sin^2 u/2}}{\sqrt{1 + \sin^2 u/2}} \simeq 2\pi A \text{Log } n + 2\pi(\gamma + \frac{3}{2} \text{Log } 2) A$$

where  $\gamma = 0.577$  is Euler's constant; thus :

$$V_{\rho\rho'} = -2\pi A \text{Log } r_{\rho\rho'}/a - 2\pi(\gamma + \frac{3}{2} \text{Log } 2) A \quad (r_{\rho\rho'} \text{ large}) \quad (4.13c)$$

An interpolation formula between (4.13b and c), accurate within 3%, is [16] :

$$V_{\rho\rho'} = -(2\pi A \text{Log } r_{\rho\rho'}/a + \pi^2 A) \quad (r_{\rho\rho'} \neq 0). \quad (4.14)$$

The Hamiltonian becomes :

$$\mathcal{H}_v \simeq -\sum_{\rho\rho'} 2\pi A q_\rho q_{\rho'} \text{Log } \frac{r_{\rho\rho'}}{a} + \pi^2 A \sum_\rho q_\rho^2.$$

At low  $T$ ,  $A = J$  according to eq. (2.11) and eq. (54) and (57) of reference [15] are recovered.

The above equations give average values, correlation functions, etc., but *not* the partition function. The calculation of the partition function is not difficult but : i) the additive constants in (2.4) and (2.5) should not be dropped; ii) the factor  $2\sqrt{\pi\beta\varepsilon}$  in (2.15) should not be dropped; iii) the contribution of the second term in (4.1) should be considered : it is easy because the  $p_\rho$ 's can be considered as continuous in the limit  $\varepsilon \rightarrow 0$ . All these contributions are regular functions of  $T$ .

4.3 EFFECT OF THE VORTICES ON THE SPINS. — If one wishes to calculate the spin pair correlation function, which is the task of Section 5, one has to calculate the following quantity which appears in eq. (3.10) :

$$\psi_k = -2\pi i \sum_\alpha A_x K_x n_{kx} \left( \sum_\alpha A_x K_x^2 \right). \quad (4.15)$$

The limit  $\varepsilon = 0$  has been taken.

Since the  $p_\rho$ 's defined by (4.2) and (4.5) do not appear in the hamiltonian (4.7), they are expected to be non-physical and therefore, if one writes the following equation, in principle easily deduced from (4.15), (4.2), (4.3) :

$$\psi_i = \sum_\rho \tilde{\Phi}_{i\rho} q_\rho + \sum_\rho \tilde{\Psi}_{i\rho} p_\rho \quad (4.16)$$

it is expected that the second term vanishes. Actually, it does not but one can take advantage of the fact that all functions of  $\psi_i$  which have a physical meaning are

periodic with period  $2\pi$ , and replace (4.16) by an equation valid modulo  $2\pi$ , namely :

$$\psi_i = \sum_{\rho} \Phi_{i\rho} q_{\rho} \quad (\text{mod. } 2\pi). \quad (4.17)$$

The derivation of this expression, which does *not* depend on the  $p$ 's, is tedious and can be found in Appendix B. It is also shown in this appendix that if the distance  $r_{i\rho}$  between  $i$  and  $\rho$  is large :

$$\Phi_{i\rho} = (\mathbf{Ox}, \mathbf{r}_{i\rho}) \quad (r_{i\rho} \gg a) \quad (4.18)$$

is the angle of  $\mathbf{r}_{i\rho} = \mathbf{R}_i - \mathbf{R}_{\rho}$  with a fixed direction  $\mathbf{Ox}$ .

Eq. (4.17) and (4.18) can be more easily derived from the qualitative picture of Kosterlitz and Thouless [15]. Finally, the model of these authors is completely recovered, except that  $J$  has to be replaced by  $A$  — a quantitative correction, which is small at low  $T$ , and amounts to 38% at  $T_c$ .

**5. Spin pair correlations in the two-dimensional isotropic planar magnet.** — 5.1 FACTORISATION OF THE SPIN PAIR CORRELATION FUNCTION. — The case  $B = 0$ , which will be considered in this section, has been extensively treated by Kosterlitz and Thouless [15] and by Kosterlitz [16], and we shall only summarize their results and show that the improvement of their method, that we have introduced, gives a quantitative agreement at low  $T$  with the Hartree approximation of Pokrovskii and Uimin [17].

Since the variables  $\theta_k$  and  $n_k^z$  are independent, the spin pair correlation function :

$$\langle \cos(\varphi_i - \varphi_j) \rangle = \langle \exp i(\varphi_i - \varphi_j) \rangle$$

can be decoupled as follows :

$$\begin{aligned} \langle \exp i(\varphi_i - \varphi_j) \rangle &= \\ &= \langle \exp i(\theta_i - \theta_j) \rangle \langle \exp i(\psi_i - \psi_j) \rangle. \end{aligned} \quad (5.1)$$

The first factor is well known :

$$\langle \exp i(\theta_i - \theta_j) \rangle \simeq \left( \frac{r_{ij}}{a} \right)^{-K_B T / 4\pi A} \quad (5.2)$$

so that the problem reduces to the calculation of the second factor in (5.1).

**5.2 THE PHASE TRANSITION OF THE 2-D ELECTROLYTE.** — Whereas the 3-D electrolyte exhibits no phase transition, as is well known, the existence of a phase transition in the classical, 2-D electrolyte has been shown in a beautiful paper by Hauge and Hemmer [18], at least in the absence of a hard core. Above a critical temperature  $T_c$ , the dielectric constant is infinite as in any well-behaved electrolyte, and can be calculated by an approximation of the Debye, or R.P.A. type, as discussed in a recent paper by Deutsch and Lavaud [19]; below  $T_c$ , pairs of opposite charges are formed, and, since they constitute neutral

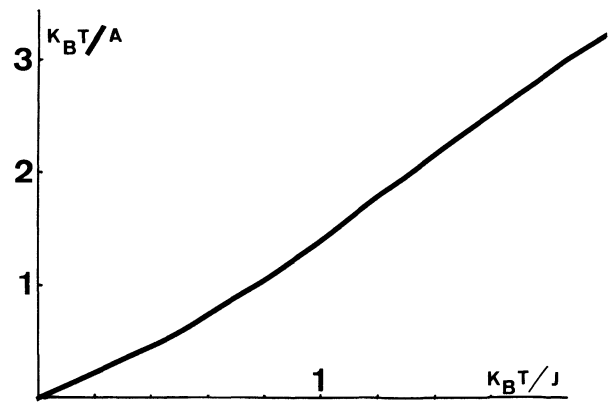


FIG. 3. — The exponent  $T/A$  of the pair correlation function (5.2) as a function of temperature.

units, the system becomes insulator. The conductor-insulator transition is still present if there is a hard core repulsion [15, 16, 19] because at low  $T$  the polarizability is given by the mean square radius of the pairs, which is finite [15], whereas at high  $T$ , R.P.A. applies and produces an infinite polarizability, as in any well-behaved electrolyte.

Thus, the equivalence of the 2-D planar magnet with a 2-D classical electrolyte (clearly shown in the present paper) yields a very convincing proof of the existence of a phase transition (disputed by Yamaji and Kondo [9]) in the 2-D planar magnet; this proof is perhaps simpler than the proof given by Berezinskii and Blank [5], which is quite convincing too.

It is of some interest to give a numerical evaluation of  $T_c$ , although comparison with experiment is difficult because real 2-D systems have marked quantum properties.  $T_c$  is given by eq. (3.5) of reference [16], where  $J$  is replaced by  $A$  :

$$\frac{A}{2 K_B T_c} = \frac{1}{2\pi} + \exp(-\pi^2 A / K_B T_c).$$

For more precision,  $\pi^2$  is replaced by

$$2\pi(\gamma + \frac{3}{2} \text{Log } 2) = 10.1595,$$

yielding :

$$K_B T_c = 2.728 A = 1.7 J = 1.7 J s^2.$$

This value is much lower than Kosterlitz' result  $2.7 J s^2$  as well as the S.C.H.A. result [14, 17],

$$2 z J s^2 / e = 2.95 J s^2,$$

but is in quite good agreement with Stanley's prediction [20] from high temperature series. We believe that our result is more reliable, however. For the Heisenberg model, a plausible approximation is obtained if  $s^2$  is replaced by  $\langle S_x^2 + S_y^2 \rangle = 2 s^2 / 3$ , yielding, in good agreement with Stanley and Kaplan [1]

$$K_B T_c \approx 1.1 J s^2.$$

This value fits the experimental data quantitatively (2%) in the reasonably *classical* example of ( $s = \frac{3}{2}$ )  $\text{Ca}_2\text{MnO}_4$  [21], whereas the fit with experiment is qualitative for  $\text{K}_2\text{NiF}_4$  [6] ( $s = 1$ ) and bad in  $\text{K}_2\text{CuF}_4$  [7] ( $s = \frac{1}{2}$ ,  $T_c \approx J/2$ ).

5.3 REGION ABOVE  $T_c$ . — For  $T > T_c$ , the equivalence with the classical electrolyte is of little help for the investigation of the 2-D planar magnet, because the quantity of interest (the second factor in (5.1)) is difficult to calculate by standard theories like R.P.A.; for instance, a cumulant expansion limited to first order :

$$\langle \exp i(\psi_i - \psi_j) \rangle = \exp -\frac{1}{2} \langle (\psi_i - \psi_j)^2 \rangle \quad (?) \quad (5.3)$$

would be a very bad approximation above  $T_c$  because the resulting spin pair correlation would not decay exponentially with  $r_{ij}$ .

However, Kosterlitz has shown [16] that there is a characteristic length which is an exponential function of  $1/(T - T_c)$ , which corresponds to a critical exponent

$$\nu = \infty$$

and therefore  $\gamma = \infty$ , in contradiction with Betts [22], who obtains for  $s = \frac{1}{2}$ , on the basis of high temperature expansions :

$$\gamma \approx 1.5.$$

In the absence of any calculation of the spin pair correlation function, it is not obvious that there is only one characteristic length, and that the length obtained by Kosterlitz is the one of interest for magnetic problems. On the other hand, investigation of critical properties by means of high temperature expansions seems difficult in 2-D isotropic systems [9, 16].

5.4 CRITICAL REGION. — The spin pair correlation function at  $T_c$  has been calculated by Kosterlitz [16], who finds critical exponents :

$$\eta = \frac{1}{4}, \quad \delta = 15$$

just as in the 2-D Ising model, and again in contradiction with Betts [22] who finds :

$$\delta \approx 5.$$

So far as we could see from Kosterlitz' calculation, the dielectric constant is not infinite at  $T_c$ , but only above  $T_c$ .

5.5 REGION BELOW  $T_c$ . — For  $T < T_c$ , it can be shown that [15, 16] :

$$\langle \exp i(\psi_i - \psi_j) \rangle \sim (r_{ij}/a)^{-\tau}. \quad (5.4)$$

It follows from (5.2) that :

$$\langle \exp i(\varphi_i - \varphi_j) \rangle \sim (r_{ij}/a)^{-\tau} \quad (5.5)$$

where

$$\tau = K_B T/4 \pi A + \tau'. \quad (5.6)$$

The power law (5.5) is similar to those derived by other methods [10, 11, 12, 14], but the present derivation is more reliable, since the potential has been replaced by an approximate potential which has the same symmetry as the original potential.

We now give an elementary derivation of (5.4), correct sufficiently below  $T_c$ .

At low  $T$ , vortices are paired and the interactions between pairs can be neglected because their distance is very large. If pairs do not interact, the probability law of  $(\psi_i - \psi_j)$  is gaussian because of the central limit theorem <sup>(1)</sup> and therefore (5.3) is correct. Insertion of (4.17) yields :

$$\langle \exp i(\psi_i - \psi_j) \rangle = \exp -\frac{1}{2} \sum_{\rho\rho'} \times (\Phi_{i\rho} - \Phi_{j\rho} - \Phi_{i\rho'} + \Phi_{j\rho'})^2 \langle q_\rho q_{\rho'} \rangle \quad (5.7)$$

where the equation :

$$\sum_{\rho'} \langle q_\rho q_{\rho'} \rangle = 0$$

has been used. For non-interacting pairs :

$$\langle q_\rho q_{\rho'} \rangle = 2 e^{2\beta V_{\rho\rho'}} \quad (5.8)$$

it is easily seen that the dominant contribution to (5.7) comes from  $r_{\rho\rho'} \ll r_{i\rho} \ll r_{ij}$  (resp.  $r_{\rho\rho'} \ll r_{j\rho} \ll r_{ij}$ ), so that the factor  $(\Phi_{i\rho} - \Phi_{j\rho} - \Phi_{i\rho'} + \Phi_{j\rho'})^2$  can be replaced by  $(r_{\rho\rho'}/2 r_{i\rho})^2$  (resp.  $r_{\rho\rho'}/2 r_{j\rho}^2$ ). Insertion of (5.8) and (4.14) into (5.7) yields eq. (5.4), with :

$$\tau' = \frac{\pi^2}{2} \frac{e^{-2\beta\pi^2 A}}{\pi\beta A - 1} \quad (5.9)$$

This formula is consistent with a transition at :

$$K_B T_c = \pi A \approx 2 J. \quad (5.10)$$

As discussed by Kosterlitz and Thouless [15], this value is reasonable, since the correct value calculated above is 1.7  $J$ , but eq. (5.9) does not describe the correct critical behaviour of  $\tau'$ . A more careful calculation [16] shows that  $\tau$  remains finite at  $T_c$ . However, (5.9) is quite correct at low  $T$  and can be used to see at which temperature  $\tau'$  becomes important in (5.6). Using (5.10) and (5.9), it is found that for  $T < 0.9 T_c$ ,  $\tau'$  can be neglected in (5.6) with an accuracy of 10%.

In this region,  $A$  is reasonably well approximated by a linear function of  $T$ , eq. (2.11), and insertion into (5.6) yields :

$$\tau = \frac{K_B T}{4 \pi J} + \frac{1}{\pi} \left( \frac{K_B T}{4 J} \right)^2 + \dots \quad (5.11)$$

<sup>(1)</sup> This is only true if  $\psi_i$  is defined by (4.17), where  $\Phi_{i\rho}$  is a smooth function of  $\mathbf{r}_{i\rho}$ , as shown in Appendix B; if definition (4.15) is used,  $\psi_i$  is singular and the central limit theorem does not apply: actually the right hand side of (5.3) is infinite at all  $T$ .



in agreement, to lowest order in  $T$ , with the Self Consistent Harmonic Approximation of Pokrovskii and Uimin. One notices that  $\tau'$  is not analytic at  $T = 0$  and cannot be accounted for in an expansion of the above type. A final remark is that a correct calculation [16] shows that  $\tau'$  can be neglected in (5.11) with an acceptable accuracy at all  $T \leq T_c$ .

**6. Discussion.** — *a)* It is not perfectly obvious that the problem defined by (2.1, 4, 5) is strictly equivalent to the problem defined by (2.1, 2, 3). This might be the reason why the critical exponents obtained from series expansions for the latter problem are different from those obtained by Kosterlitz for the former problem. We believe, however, that both problems are strictly equivalent (apart from obvious quantitative differences), and we try to justify this statement below.

A first remark is that the high temperature series expansions using model (1.1, 2, 3) seem to be consistent with an infinite value of  $\gamma$  (Camp and Van Dyke, preprint).

*b)* An alternative way of writing (2.6) is a sum of a bilinear exchange term similar to (2.2), plus a biquadratic exchange, etc. In addition the coupling constants are functions of  $T$ , but these functions are analytic, so that this fact cannot influence the critical exponents. Now, the existence of biquadratic and higher terms is not expected to modify the nature of the order below  $T_c$  nor the critical exponents, provided the Universality Principle is admitted : both problems (2.1, 4, 5) and (2.1, 2, 3) are obviously represented by the same type of Landau-Wilson free energy.

*c)* However, since the Universality Principle cannot be considered as a proof, one wishes to improve the approximation (2.4) of the original potential (2.2) : the next approximation is given by (2.18) ; in this approximation, the vortex hamiltonian (4.7) is replaced if (4.9) holds by :

$$\mathcal{H} = \sum_k \frac{A}{K^2} [4 \pi^2 |q_k|^2 + 2 \pi i \alpha q_k^* (K_y S_k^x - K_x S_k^y) + h.c. + \alpha^2 |K_y S_k^x - K_x S_k^y|^2].$$

A simple way to account for the additional terms is to assume a linear law :

$$i(K_y S_k^x - K_x S_k^y) = -2 \pi \alpha q_k \chi_k^s \quad (6.2)$$

so that (4.7) is recovered, except that  $A$  must be replaced by  $A(1 - 2 \alpha^2 \chi_k^s + \alpha^2 \chi_k^{s2})$  and the results are essentially unchanged. The susceptibility  $\chi_k^s$  of the

spin system cannot be easily calculated but it is fairly clear that it has no singularity. Of course the linear law (6.2) is only valid in the limit  $\alpha \rightarrow 0$ , and the effect of possible higher order terms in (6.2) is difficult to evaluate. It is reasonable, however, to speculate that they are not essential.

*d)* Finally, the same exponents as obtained by Kosterlitz can be derived in a quite different (but not rigorous) way : the 2D, classical,  $X - Y$  model can be transformed by a functional integration technique into an  $XY$  chain of spin 1 at  $T = 0$  in a transverse anisotropy field (which depends on the temperature  $T$  of the original 2-D problem). If one approximates the latter problem by an  $XY$  chain of spin 1/2 in a transverse field (a rigorously soluble problem) one finds  $\alpha = -\infty$  and therefore, if one accepts scaling laws :  $D\nu = 2 - \alpha$  and  $\nu = +\infty$ , in agreement with Kosterlitz. Thus, there is a strong theoretical support in favour of the result  $\nu = \infty$ , and probably

$$\gamma = (2 - \eta) \nu = \infty.$$

*e)* However, recently published experimental data yield a finite value  $\gamma = 2.37$  for the 2-D  $XY$  model, although it is much larger than Betts' prediction [23, 24].

*f)* In the absence of any calculation of the spin pair correlation function above  $T_c$  in the model (2.1, 4, 5), one can have no idea of the temperature region where the divergence of the critical exponents becomes significant.

**7. Conclusion.** — Our method provides a more quantitative basis to the Kosterlitz-Thouless theory of the 2-D planar magnet, and suggests substantial corrections : for instance, the critical temperature is lowered by about 40 %. It is confirmed that the spin pair correlation function behaves like a power law below  $T_c$ , and the exponent coincides at low  $T$  with the prediction of the self consistent harmonic approximation ; however, the discrepancy with S.C.H.A. becomes important near  $T_c$  : for instance the value predicted for  $T_c$  is twice as small as in S.C.H.A. Our value of  $T_c$  compares favourably with experiment, but a precise comparison is impossible because of quantum effects, which we have neglected. More detailed comparison with experiment will be made in a subsequent paper, devoted to more realistic models with an anisotropy.

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## APPENDIX A

One wishes to approximate the function :

$$f(u) = e^{\epsilon \cos u} \quad (A 1)$$

by an expression of the form :

$$Rg(u) = R \sum_{n=-\infty}^{\infty} \exp - \gamma(u - 2 \pi n)^2 \quad (A 2)$$

where  $R$  and  $\gamma$  are constants and  $n$  is an integer. In the notations of Section 2; one has

$$\varepsilon = 2 \beta J_{ij} \quad \text{or} \quad \varepsilon = \beta D \quad (\text{A } 3)$$

and

$$\gamma = \beta A_{ij} \quad \text{or} \quad \gamma = \beta B. \quad (\text{A } 4)$$

According to the prescription of Section 2, the first 2 Fourier components of (A 1) and (A 2) must be the same. The Fourier series for  $g(u)$  is :

$$g(u) = \sum_{m=-\infty}^{\infty} b_m e^{imu} \quad (\text{A } 5)$$

with

$$\begin{aligned} b_m &= \frac{1}{2\pi} \int_{-\pi}^{\pi} du e^{-imu} \sum_{n=-\infty}^{\infty} e^{-\gamma(u-2\pi n)^2} \\ &= \int_{-\pi}^{\pi} du e^{-imu} \sum_{n=-\infty}^{\infty} e^{-\gamma(u-2\pi n)^2} \\ &= \int_{-\infty}^{\infty} dv e^{-\gamma v^2 - imv} \\ b_m &= \frac{e^{-m^2/4\gamma}}{2\sqrt{\pi\gamma}}. \end{aligned} \quad (\text{A } 6)$$

On the other hand the Fourier series for (A 1) is

$$f(u) = \sum_{m=-\infty}^{\infty} a_m e^{imu} \quad (\text{A } 7)$$

with :

$$\begin{aligned} a_m &= \frac{1}{2\pi} \int_{-\pi}^{\pi} du e^{\varepsilon \cos u} e^{-imu} \\ &= i^{-m} J_m(i\varepsilon) = I_m(\varepsilon) \end{aligned} \quad (\text{A } 8)$$

where  $I_n$  is a modified Bessel function.

If (A 2) is wished to approximate (A 1), one must have :

$$a_0 = Rb_0, \quad a_1 = Rb_1.$$

Eliminating  $R$ , one gets from (A 6) and (A 8) :

$$e^{-1/4\gamma} = I_1(\varepsilon)/I_0(\varepsilon) = a_1/a_0. \quad (\text{A } 9)$$

a) For large  $\varepsilon$  (low  $T$  limit)

$$\begin{aligned} a_m &\simeq \exp\left(\varepsilon - \frac{m^2}{2\varepsilon}\right) \times \\ &\quad \times \left(1 + \frac{1}{8\varepsilon} + \frac{1}{24\varepsilon^2} - \frac{m^2}{4\varepsilon^2} + \dots\right) \end{aligned}$$

and (A 9) reads :

$$\gamma = \frac{\varepsilon}{2} \left(1 - \frac{1}{2\varepsilon}\right) \quad (\text{A } 10)$$

b) For small  $\varepsilon$  (high  $T$  limit)

$$a_0 \simeq 1 \quad a_1 \simeq \varepsilon/2$$

and (A 9) reads :

$$\exp\left(-\frac{1}{4\gamma}\right) = \frac{\varepsilon}{2}$$

and (A 9) reads :

$$\gamma = \frac{1}{4 \text{Log} \frac{2}{\varepsilon}}. \quad (\text{A } 11)$$

Insertion of (A 3, 4) into (A 10, 11) yields eq. (2.9, 10, 11).

### APPENDIX B

The Fourier transform of (4.15) can, using (3.1c), be written as :

$$\psi_i \equiv \frac{1}{\sqrt{N}} \psi_k e^{-i\mathbf{k} \cdot \mathbf{R}_i} \quad (\text{B } 1)$$

$$\begin{aligned} \psi_i &= -\frac{2\pi i}{N} \sum_{l < m} \sum_{\alpha} n_{lm}^{\alpha} \sum_k \frac{A_{\alpha} K_{\alpha}}{\sum_{\xi} A_{\xi} K_{\xi}^2} \times \\ &\quad \times \exp\left[i\mathbf{k} \cdot \left(\frac{\mathbf{R}_l + \mathbf{R}_m}{2} - \mathbf{R}_i\right)\right]. \end{aligned} \quad (\text{B } 2)$$

It is convenient to express  $\psi_i$  in terms of the  $p_{\rho}$ 's and  $q_{\rho}$ 's in the case when all  $n_{ij} = 0$  except for one single bond. If an equation which has the same form for all bonds horizontal or vertical is obtained, and if it is linear, it can be easily extended to any number of bonds with  $n_{ij} \neq 0$ .

i) If all  $n_{ij} = 0$  except on one vertical bond, the

following expression can be deduced after some manipulation from (B 1) and (4.4) :

$$\psi_i = \sum_{\rho} Y_{i\rho} q_{\rho} \quad (\text{B } 3)$$

with :

$$Y_{i\rho} = \frac{2\pi}{N} \sum_k \frac{K_y}{K_x} \frac{e^{i\mathbf{k} \cdot (\mathbf{R}_{\rho} - \mathbf{R}_i)}}{K_x^2 + K_y^2}. \quad (\text{B } 4)$$

The assumption (4.9) has been used. (B 3) also holds if  $n_{ij} = 0$  except on any number of vertical bonds, since it is linear.

ii) If all  $n_{ij} = 0$  except on one horizontal bond, the corresponding relations are :

$$\psi_i = \sum_{\rho} X_{i\rho} q_{\rho} \quad (\text{B } 5)$$

$$X_{i\rho} = -\frac{2\pi}{N} \sum_k \frac{K_x}{K_y} \frac{e^{i\mathbf{k} \cdot (\mathbf{R}_{\rho} - \mathbf{R}_i)}}{K_x^2 + K_y^2}. \quad (\text{B } 6)$$

A unified form is wanted instead of the 2 relations (B 3) and (B 5). For this purpose, (B 5) can be replaced by :

$$\psi_i = \sum_{\rho} Y_{i\rho} q_{\rho} + \sum_{\rho} (X_{i\rho} - Y_{i\rho}) q_{\rho} \quad (\text{B } 7)$$

where, from (B 4) and (B 6) :

$$X_{i\rho} - Y_{i\rho} = -\frac{2\pi}{N} \sum_k \frac{e^{ik \cdot (\mathbf{R}_{\rho} - \mathbf{R}_i)}}{K_x K_y} = -2\pi \gamma_x(x_{i\rho}) \gamma_y(y_{i\rho})$$

where  $x_{i\rho}$  and  $y_{i\rho}$  are the components of  $(\mathbf{R}_{\rho} - \mathbf{R}_i)$  and the function :

$$\gamma_x(x) = \frac{1}{N_x} \sum_{k_x} \frac{e^{ik_x x}}{K_x}$$

satisfies the relations :

$$\begin{aligned} \gamma_x(x) &= \gamma_x(-x) \\ \gamma_x(x) - \gamma_x(x-a) &= \delta_{x,a/2} \end{aligned}$$

Hence :

$$\gamma_x(x) = \gamma_y(x) = \frac{1}{2} \frac{x}{|x|}$$

and :

$$X_{i\rho} - Y_{i\rho} = \begin{cases} -\pi/2 & \text{if } x_{i\rho} y_{i\rho} > 0 \\ \pi/2 & \text{if } x_{i\rho} y_{i\rho} < 0. \end{cases} \quad (\text{B } 8)$$

In the case when all  $n$ 's vanish except on one horizontal bond, it can be shown by inspection that (B 7) and (B 8) can be replaced by :

$$\psi_i = \sum_{\rho} (Y_{i\rho} q_{\rho} + F_{i\rho} q_{\rho}) \pmod{2\pi} \quad (\text{B } 9)$$

with

$$\left. \begin{aligned} F_{i\rho} &= -\pi/2 \pmod{2\pi} \quad \text{if } y_{\rho} < y_i \\ F_{i\rho} &= +\pi/2 \pmod{2\pi} \quad \text{if } y_{\rho} > y_i \end{aligned} \right\} \quad (\text{B } 10)$$

The advantage of (B 9) over (B 7) is that it can be seen by inspection that if all  $n$ 's vanish except for one vertical bond, (B 3) can also be replaced by (B 9). Since (B 9) applies for one horizontal bond or one vertical bond and since it is linear, it is perfectly general and applies to all values of the  $n_{ij}$ 's.

Expression of  $\psi_i$  far from vortices. — We now wish to find an approximate form of (B 9) when all

$$\mathbf{r}_{i\rho} = \mathbf{R}_{\rho} - \mathbf{R}_i$$

are large. In this case  $K_x$  and  $K_y$  can be replaced by  $k_x$  and  $k_y$  in (B 4), and therefore : the function :

$$Y_{i\rho} = Y(\mathbf{r}_{i\rho})$$

satisfies :

$$\begin{aligned} \frac{\partial Y(\mathbf{r})}{\partial x} &= \frac{2\pi_i}{N} \sum_k \frac{k_y}{k^2} e^{ik \cdot \mathbf{r}} \\ &= \frac{2\pi}{N} \frac{\partial}{\partial y} \sum_k \frac{e^{ik \cdot \mathbf{r}}}{k^2} \\ &= -\frac{2\pi}{N} \frac{\partial}{\partial y} \sum_k \frac{1 - e^{ik \cdot \mathbf{r}}}{k^2} \\ &= -\frac{\partial}{\partial y} \text{Log} \frac{r}{a} \\ &= -y/r^2 \\ &= +\partial\Phi/\partial x \end{aligned} \quad (\text{B } 11)$$

where  $\Phi = (Ox, r)$  is the polar angle of  $r$ . Integration of (B 11) yields :

$$Y(r) = \Phi + f(y) \quad (\text{B } 12)$$

where  $f(y)$  is a function of  $y$ . Similarly :

$$X(r) = \Phi + g(x) \quad (\text{B } 13)$$

Insertion of (B 12) and (B 13) into (B 8) shows that

$$\begin{aligned} f(y) &= \pi/2 + C \quad \text{if } y < 0 \\ f(y) &= -\pi/2 + C \quad \text{if } y > 0 \end{aligned} \quad (\text{B } 14)$$

where the constant  $C$  disappears from all physical problems and will not be precised. If (B 12) and (B 14) are inserted into (B 9)  $f(y)$  cancels  $F_{i\rho}$  and (B 9) reads :

$$\psi_i = \sum_{\rho} \Phi_{i\rho} q_{\rho} \pmod{2\pi} \quad (\text{B } 15)$$

where  $\Phi_{i\rho} = (O\mathbf{x}, \mathbf{r}_{i\rho})$  is the polar angle of  $\mathbf{r}_{i\rho}$ .

Eq. (B 15) can be derived in a much simpler way in the model of Kosterlitz and Thouless [15].

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