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Ordering, metastability and phase transitions in two-dimensional systems

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Abstract. A new definition of order called topological order is proposed for two-dimensional systems in which no long-range order of the conventional type exists. The possibility of a phase transition characterized by a change in the response of the system to an external perturbation is discussed in the context of a mean field type of approximation. The critical behaviour found in this model displays very weak singularities. The application of these ideas to the xy model of magnetism, the solid–liquid transition, and the neutral superfluid are discussed. This type of phase transition cannot occur in a superconductor nor in a Heisenberg ferromagnet, for reasons that are given.

1. Introduction

Peierls (1935) has argued that thermal motion of long-wavelength phonons will destroy the long-range order of a two-dimensional solid in the sense that the mean square deviation of an atom from its equilibrium position increases logarithmically with the size of the system, and the Bragg peaks of the diffraction pattern formed by the system are broad instead of sharp. The absence of long-range order of this simple form has been shown by Mermin (1968) using rigorous inequalities. Similar arguments can be used to show that there is no spontaneous magnetization in a two-dimensional magnet with spins with more than one degree of freedom (Mermin and Wagner 1966) and that the expectation value of the superfluid order parameter in a two-dimensional Bose fluid is zero (Hohenberg 1967).

On the other hand there is inconclusive evidence from the numerical work on a two-dimensional system of hard discs by Alder and Wainwright (1962) of a phase transition between a gaseous and solid state. Stanley and Kaplan (1966) found that high-temperature series expansions for two-dimensional spin models indicated a phase transition in which the susceptibility becomes infinite. The evidence for such a transition is much stronger for the xy model (spins confined to a plane) than for the Heisenberg model, as can be seen from the papers of Stanley (1968) and Moore (1969). Low-temperature expansions obtained by Wegner (1967) and Berezinskii (1970) give a magnetization proportional to some power of the field between zero and unity, and indicate the possibility of a sharp transition between such behaviour and the high-temperature régime where the magnetization is proportional to the applied field.

In this paper we present arguments in favour of a quite different definition of long-range order which is based on the overall properties of the system rather than on the

behaviour of a two-point correlation function. In the cases we consider, the usual correlation function, such as the spin–spin correlation function, vanishes at any finite temperature in contrast to the corresponding cases in three dimensions. This type of long-range order, which we refer to as topological long-range order, may exist for the two-dimensional solid, neutral superfluid, and for the xy model, but not for a superconductor or isotropic Heisenberg model. In the case of a solid, the disappearance of topological long-range order is associated with a transition from an elastic to a fluid response to a small external shear stress, while for a neutral superfluid it is associated with the instability of persistent currents. Recently, Berezinskii (1971) has put forward similar arguments, but there are some important differences in our results. A brief account of this theory has already been given (Kosterlitz and Thouless 1972).

The definition of long-range order which we adopt arises naturally in the case of a solid from the dislocation theory of melting (Nabarro 1967). In this theory, it is supposed that a liquid close to its freezing point has a local structure similar to that of a solid, but that in its equilibrium configurations there is some concentration of dislocations which can move to the surface under the influence of an arbitrarily small shear stress, and so produce viscous flow. In the solid state there are no free dislocations in equilibrium, and so the system is rigid. This theory is much easier to apply in two dimensions than in three since a dislocation is associated with a point rather than a line.

Although isolated dislocations cannot occur at low temperatures in a large system (except near the boundary) since their energy increases logarithmically with the size of the system, pairs of dislocations with equal and opposite Burgers vector have finite energy and must occur because of thermal excitation. Such pairs can respond to an applied stress and so reduce the rigidity modulus. At sufficiently high temperatures, the largest pairs become unstable under an applied shear stress and produce a viscous response to the shear.

The presence or absence of free dislocations can be determined in the following manner. We suppose that the system has a fair degree of short-range order so that a local crystal structure can be identified. To be definite we take the crystal structure to be a simple square lattice with spacing $\boldsymbol{a}$. Using the local order, we attempt to trace a path from atom to atom which, in the perfect crystal, would be closed. Mermin (1968) has commented that the thermal motion does not necessarily destroy the correlation in orientation of the crystal axes at large distances, but even if this is destroyed, the direction taken in one region can be defined in terms of that taken in a previous region in the same neighbourhood. Local defects can be avoided by small deformations of the path. This procedure is possible provided there are no grain boundaries. If there are free dislocations present, the number of dislocations contained within the region surrounded by the contour will be proportional to the area of the region. Since the Burgers vectors of the individual dislocations can point in two possible directions, the average total Burgers vector will be proportional to the square root of the area. The path will fail to close by an amount proportional to L, the length of the path. If there are only pairs of dislocations present, only those pairs which are cut by the contour will contribute to the total Burgers vector. The number of pairs cut by the path is proportional to Lr where r is the mean separation of the pairs. Averaging over the possible orientations of the individual Burgers vectors, we see that the path will fail to close by an amount proportional to $(Lr)^{1/2}$. This allows us to determine the presence or absence of topological long-range order in the system.

We can obtain estimates of the transition temperature for the systems discussed by arguments similar to those used by Thouless (1969) for a one-dimensional Ising model

with an interaction falling off at large distances as r^{-2}. At large distances from a dislocation (or vortex in the case of the xy model and neutral superfluid) the strain produced is inversely proportional to the distance and so the energy of a single dislocation depends logarithmically on the size of the system. In fact, the energy of an isolated dislocation with Burgers vector of magnitude b in a system of area A is (Friedel 1964)

$$E = \frac{vb^2(1+\tau)}{4\pi} \ln \frac{A}{A_0} \tag{1}$$

where v and τ are the two-dimensional rigidity modulus and Poisson's ratio respectively, and A_0 is an area of the order of b^2. The entropy associated with a dislocation also depends logarithmically on the area, and, since there are approximately A/A_0 possible positions for the dislocation, the entropy is

$$S = k_B \ln \frac{A}{A_0} + O(1) \tag{2}$$

where k_B is the Boltzmann constant.

Since both energy and entropy depend on the size of the system in the same way, the energy term will dominate the free energy at low temperatures, and the probability of a single dislocation appearing in a large system will be vanishingly small. At high temperatures, dislocations will appear spontaneously when the entropy term takes over. The critical temperature at which a single dislocation is likely to occur is the temperature at which the free energy changes sign, namely (Kosterlitz and Thouless 1972)

$$k_B T_c = \frac{vb^2(1+\tau)}{4\pi} \tag{3}$$

Identical considerations for the xy model give

$$k_B T_c = \pi J \tag{4}$$

where J is the spin–spin coupling constant and

$$k_B T_c = \frac{\pi \hbar^2 \rho}{2m} \tag{5}$$

for the neutral superfluid where ρ is the density of particles per unit area and m is the effective atomic mass which is not necessarily the same as the atomic mass for a particle moving on a substrate.

That these estimates are upper bounds can be seen by the following argument. Although the formation of isolated dislocations will not occur at low temperatures, there can always be production of a pair of dislocations with equal and opposite Burgers vector, since the strain produced by such a pair falls off sufficiently rapidly at large distances so that the energy is finite. The critical temperatures as calculated above are the temperatures at which a pair of dislocations (or vortices) will dissociate, ignoring the effect of other pairs in the system. These other pairs will relax in the field of the first pair thereby renormalizing the rigidity modulus etc. downwards and consequently reducing the critical temperature. Most of the rest of the paper is devoted to a detailed study of this phenomenon in the systems discussed.

2. A model system

The statistical problem we are faced with is essentially that of a two-dimensional gas of particles with charges $\pm q$ interacting via the usual logarithmic potential, the number of particles being constrained only by the requirement that the system has overall electrical neutrality. The only essential modification necessary to treat the dislocation problem is to allow for the two different possible orientations of the Burgers vector. The hamiltonian for such a system is

$$H(\boldsymbol{r}_1 \ldots \boldsymbol{r}_N) = \tfrac{1}{2} \sum_{i \neq j} U(|\boldsymbol{r}_i - \boldsymbol{r}_j|) \tag{6}$$

where

$$\begin{aligned} U(|\boldsymbol{r}_i - \boldsymbol{r}_j|) &= -2q_i q_j \ln \left| \frac{\boldsymbol{r}_i - \boldsymbol{r}_j}{r_0} \right| + 2\mu \qquad r > r_0 \\ &= 0 \qquad\qquad\qquad\qquad\qquad\quad r < r_0 . \end{aligned}$$

Here q_i and $\boldsymbol{r}_i$ are the charge and position of the ith particle, 2μ is the energy required to create a pair of particles of equal and opposite charge a distance r_0 apart, and r_0 is some suitable cutoff to avoid spurious divergences at small separations. We expect that the cutoff r_0 is of the order of the particle diameter or, for a lattice, the lattice spacing. In such a lattice near the critical point, we will be able to replace sums over the lattice sites by an integral over the whole system since the important contributions to the sum will come from the long-range part of the interaction, that is $|\boldsymbol{r}_i - \boldsymbol{r}_j| \gg r_0$.

To obtain a tractable theory, we further assume that the chemical potential μ is sufficiently large that there are very few particles present in the system. Since we have such a dilute gas, the configurations of least energy are those where equal and opposite charges are closely bound in dipole pairs, well separated from one another. At low temperatures, therefore, the fluctuations of charge within a given region are restricted, while at high temperatures charges may occur in isolation so much larger fluctuations may occur. For such configurations, we see that the mean square separation of the particles making up a dipole pair (ignoring for the present interactions between the pairs) is

$$\langle r^2 \rangle = \frac{\int_{r_0}^{\infty} \mathrm{d}r\, r^3 \exp\{-2\beta q^2 \ln (r/r_0)\}}{\int_{r_0}^{\infty} \mathrm{d}r\, r \exp\{-2\beta q^2 \ln (r/r_0)\}} = r_0^2 \frac{\beta q^2 - 1}{\beta q^2 - 2} \tag{7}$$

where $\beta = 1/k_B T$. The probability of finding a pair within a given area is found by summing $\exp\{-2\beta\mu - 2\beta q^2 \ln (|\boldsymbol{r}_i - \boldsymbol{r}_j|/r_0)\}$ over all values of $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$ in the area. The double sum can be replaced by a double integral if we normalize by a factor of order r_0^{-4}, so that the mean separation d between such pairs is given in the same approximation by

$$\begin{aligned} \frac{1}{d^2} &\approx \frac{\mathrm{e}^{-2\beta\mu}}{r_0^4} \int \mathrm{d}^2 \boldsymbol{r} \exp\{-2\beta q^2 \ln (r/r_0)\} + \mathrm{O}(\mathrm{e}^{-4\beta\mu}) \\ &= \frac{\pi}{r_0^2} \mathrm{e}^{-2\beta\mu} \frac{1}{\beta q^2 - 1} . \end{aligned} \tag{8}$$

Here we can see the necessity for a large chemical potential μ, since already in calculating d^{-2}, any terms beyond first order in $\exp(-2\beta\mu)$ become intractable. Thus

$$\langle (r/d)^2 \rangle \approx \frac{\pi \mathrm{e}^{-2\beta\mu}}{\beta q^2 - 2} \ll 1 \qquad \text{for} \qquad \beta q^2 < 2 . \tag{9}$$

We can already see that a phase transition to a conducting state will take place at a temperature T_c given by

$$k_B T_c \approx \tfrac{1}{2}q^2 \tag{10}$$

since, in this simple approximation the polarizability, which is proportional to $\langle r^2 \rangle$, diverges. The closely bound dipole pairs will separate to give a uniform two-dimensional plasma of oppositely charged particles. The free energy of an isolated charge is

$$F = E - TS \approx \tfrac{1}{2}q^2 \ln (R^2/r_0^2) - k_B T \ln (R^2/r_0^2) \tag{11}$$

where R is the radius of the system. Thus we see that isolated charges can appear spontaneously when the temperature reaches T_c as given by equation (10). We are therefore particularly interested in values of βq^2 near 2.

Hauge and Hemmer (1971) have investigated the two-dimensional Coulomb gas under very different conditions. In the limit of vanishing particle size, they find a transition at $kT = q^2$ (in our units), the temperature at which pairs begin to form as $kT \to q^2$ from above. We look at a different temperature range and find a transition near $kT = \frac{1}{2}q^2$, when the largest pairs dissociate as the transition is approached from below. The main difference between the two models is the presence of a finite cutoff in this paper, which makes the potential well behaved at small distances, while Hauge and Hemmer allow the potential to be singular at the point of closest approach.

The divergence of the polarizability as the transition temperature is approached from below suggests that the most important effect of the interactions between different pairs may be described by the introduction of a dielectric constant. The field of a pair separated by a small distance of the order of r_0 does not extend much beyond the distance of separation of the two charges and from equation (8) it is very unlikely that there will be another pair in their immediate vicinity. Thus the dielectric constant appropriate for the expression of the energy of such a pair is unaffected by the polarizability of the other pairs. It is only for charges separated by an amount greater than the mean separation d of pairs that the energy is modified by the presence of other smaller pairs lying within the range of the field. The effective dielectric constant, therefore, becomes larger as we consider larger and larger pairs, so that the problem becomes a sort of iterated mean field approximation. We are therefore faced with problems similar to those which led to rescaling in the paper of Anderson *et al* (1970).

Within the range of a pair with large separation $r \gg r_0$ it is expected that there will be other pairs with separation up to $r \exp(-\beta\mu)$. The effect of these will be to reduce the interaction energy of the large pair by introducing an effective dielectric constant $\epsilon(r)$. To calculate this dielectric constant we consider pairs with separations lying in a small interval between r and $r + \mathrm{d}r$ with $\mathrm{d}r \ll r$, and consider terms to first order only in $\mathrm{d}r$. Using the standard methods of linear response theory, we apply a weak electric field E at an angle θ to the line joining the two charges. The polarizability per pair is given by

$$p(r) = q \frac{\partial}{\partial E} \langle r \cos\theta \rangle \Big|_{E=0} \tag{12}$$

where the average is taken over the annulus $r < r' < r + \mathrm{d}r$ with Boltzmann factor

$$\exp\{-\beta U(r)\} = \left(\frac{r}{r_0}\right)^{-2\beta q^2/\epsilon(r)} \exp(\beta E q r \cos\theta) . \tag{13}$$

Although formally the factor $\exp(\beta E r q \cos\theta)$ will cause a divergence in the integrals of equation (12), we can argue that we can carry out the differentiation with respect to E

and take the limit $E \to 0$ before integrating as follows. Inside the medium the effective field is set up by the two charges, and falls off rapidly at distances greater than the separation between the charges and so has a finite range. Moreover, since the dipole pairs within this field have a separation very much less than the separation of the two charges of interest, the field experienced by the dipole pairs is effectively constant over them. Thus, our method of calculating the polarizability of a given pair from equation (12) is justified. We easily obtain

$$p(r) = \tfrac{1}{2}\beta q^2 r^2. \tag{14}$$

The density of such pairs is, by the same argument that leads to equation (8),

$$\mathrm{d}n(r) = \frac{1}{r_0^4}\int_0^{2\pi} \mathrm{d}\theta \int_r^{r+\mathrm{d}r} \mathrm{d}r'\, r' \exp\{-\beta U_{\mathrm{eff}}(r')\} + \mathrm{O}(\mathrm{e}^{-4\beta\mu}) \tag{15}$$

where $U_{\mathrm{eff}}(r)$ is the energy of two charges separated by r in such a dielectric medium. The terms $\mathrm{O}(\mathrm{e}^{-4\beta\mu})$ correspond to the fact that in the normalization of the probability for seeing such pairs there are terms corresponding to seeing no pairs, one pair etc, all of which we ignore except for the no-pair term. Another complication arises at this point because the energy $U_{\mathrm{eff}}(r)$ is given by

$$U_{\mathrm{eff}}(r) = 2\mu + 2q^2 \int_{r_0}^{r} \frac{\mathrm{d}r'}{r'\epsilon(r')}\,. \tag{16}$$

As it stands, we cannot evaluate equation (16) because of the unknown function $\epsilon(r)$. However, assuming that $\mathrm{d}\epsilon^{-1}(r)/\mathrm{d}r$ is sufficiently small, we can write

$$U_{\mathrm{eff}}(r) = \frac{2q^2 \ln(r/r_0)}{\epsilon(r)} \tag{17}$$

and check the consistency of this assumption *a posteriori*. We finally obtain the susceptibility due to these pairs

$$\mathrm{d}\chi(r) = \pi\beta q^2 \mathrm{e}^{-2\beta\mu}\left(\frac{r}{r_0}\right)^{-2\beta q^2/\epsilon(r)+4} \mathrm{d}\left(\ln\frac{r}{r_0}\right). \tag{18}$$

Lastly, we change variables to

$$x = \ln\frac{r}{r_0} \qquad \text{and} \qquad y(x) = \frac{2\beta q^2}{\epsilon(x)} - 4$$

to obtain the differential equation

$$\frac{\mathrm{d}y}{\mathrm{d}y} = -\pi^2 \mathrm{e}^{-2\beta\mu}(y+4)^2\ \mathrm{e}^{-x}) \tag{19}$$

which is subject to the boundary conditions

$$y(0) = 2\beta q^2 - 4 \qquad \text{and} \qquad y(\infty) = \frac{2\beta q^2}{\epsilon} - 4 \tag{20}$$

where ϵ is the macroscopic dielectric constant. Since, as discussed previously, when $x = 0$, $r = r_0$ so that the interaction of a pair separated by r_0 is unaffected by any other pairs, so that $\epsilon(x = 0) = 1$. Similarly, as $x \to \infty$, the effective interaction is reduced by a factor $\epsilon(x = \infty)$, which must be the same as the dielectric constant as measured by application of an external field to a macroscopic region of the medium. We can simplify

equation (19) further by noticing that, since the derivative dy/dx is proportional to $e^{-2\beta\mu}$, the difference $y(0) - y(\infty)$ for $y(0) > y_c(0)$ must also be very small (in fact $y(0) - y(\infty) < O(e^{-\beta\mu})$) so that we can replace the factor $(y + 4)^2$ in equation (19) by $(y(0) + 4)^2$.

The problem is now reduced to solving the equation

$$\frac{d\tilde{y}}{d\tilde{x}} = -\exp(-\tilde{x}\tilde{y}) \tag{21}$$

where we have rescaled $x = (\pi e^{-\beta\mu}(y(0) + 4))^{-1}\ \tilde{x}$ and $y = (\pi e^{-\beta\mu}(y(0) + 4))\,\tilde{y}$ to eliminate the constant multiplying the exponential. This equation does not possess an analytic solution but the solutions fall into two classes (see Appendix)

$$\begin{aligned} &\text{(i)} && \frac{q^2}{k_B T \epsilon(T)} - 2 > 0 && \text{for } T < T_c \\ &\text{(ii)} && \frac{q^2}{k_B T \epsilon(T)} - 2 \to -\infty && \text{for } T > T_c . \end{aligned} \tag{22}$$

We interpret this sudden change in the behaviour of $\epsilon(T)$ as T passes through T_c as a phase transition to the conducting state where the pairs become unbound. The critical temperature T_c is given by

$$\frac{q^2}{k_B T_c} = 2\left[1 + \left\{\tilde{y}_c(0)\,\pi \exp\left(\frac{-\mu}{k_B T_c}\right)\right\}\right] \tag{23}$$

and the critical value of the dielectric constant at the transition temperature is given by

$$\frac{q^2}{k_B T_c} - 2\epsilon(T_c) = 0 . \tag{24}$$

To determine the values of T_c and ϵ_c and to investigate the nature of the phase transition, it is necessary to find an approximate solution of equation (21). This can be done in two limiting cases, $T \ll T_c$ and $T \lesssim T_c$. In the first case, $y(0) \approx y(\infty) > 0$ so we can immediately integrate equation (21) by replacing $y(x)$ by $y(0)$ in the exponential to obtain

$$\epsilon \approx 1 + \frac{\pi^2 \beta q^2 e^{-2\beta\mu}}{\beta q^2 - 2} . \tag{25}$$

In the second case $T \lesssim T_c$, equation (21) may be solved approximately by the methods described in the Appendix to obtain $\tilde{y}_c(0) = 1{\cdot}3$ so that

$$\frac{q^2}{k_B T_c} \approx 2\{1 + 1{\cdot}3\pi \exp(-\mu/k_B T_c)\} \tag{26}$$

and

$$\left(\frac{q^2}{k_B T \epsilon(T)} - 2\right) \underset{T \to T_c}{\sim} \exp\left\{-\left(\ln \frac{T_c}{T_c - T}\right)^{1/2}\right\} . \tag{27}$$

This singularity in $\epsilon(T)$ is of a most unusual type but, since we have used a mean field theory, this form of the singularity is unlikely to be the correct one. Note in particular that $\epsilon(T_c)$ is finite so that the susceptibility does not diverge at the critical temperature as one would expect from the simple arguments presented earlier.

We are now in a position to check our assumption that $d\epsilon^{-1}(r)/dr$ is sufficiently small to do the integration in equation (16). Clearly, for $T \ll T_c$, the replacement of $\epsilon^{-1}(r)$ by a constant is valid. The most unfavourable case is for the critical trajectory when $y(\infty) = 0$ and $d\epsilon^{-1}(r)/dr$ is largest. The condition for the replacement to be valid is

$$\frac{d\epsilon^{-1}(r)}{dr} \underset{r\to\infty}{\ll} \frac{1}{r \ln r} . \tag{28}$$

The critical solution of equation (21) is, as can be verified by direct substitution

$$\tilde{y}(x) \underset{x\to\infty}{\sim} \frac{2 \ln \tilde{x}}{\tilde{x}} - \frac{\ln \ln \tilde{x}}{\tilde{x}} + \ldots \tag{29}$$

Remembering that $\tilde{x} \propto \ln r/r_0$, this gives

$$\frac{d\epsilon^{-1}(r)}{dr} \underset{r\to\infty}{\sim} \frac{1}{r \ln r} \frac{\ln \ln r}{\ln r} \ll \frac{1}{r \ln r} . \tag{30}$$

The free energy has a singularity at the critical temperature but it is so weak that any observable except the dielectric constant is finite and all derivatives are finite and bounded for $T < T_c$. Not surprisingly, this is in agreement with the results obtained by Anderson and Yuval (1971) for the one-dimensional Ising model with inverse square interaction, which can be treated with our methods to obtain most of their results. The energy of a pair of charges is

$$U = \frac{q^2 \int_0^\infty dx\, x\, \epsilon^{-1}(x) \exp\{-2(\beta q^2 \epsilon^{-1}(x) - 1)x\}}{\int_0^\infty dx \exp\{-2(\beta q^2 \epsilon^{-1}(x) - 1)x\}} \tag{31}$$

where we have substituted $x = \ln (r/r_0)$. Since the specific heat C is proportional to $dU/d\beta$, any singularities in C will show up in integrals of the form

$$\int_0^\infty dx\, x^n \frac{\partial \epsilon^{-1}(x)}{\partial \beta} \exp\{-2(\beta q^2 \epsilon^{-1}(x) - 1)x\} \approx \int_0^\infty dx\, x^n e^{-\alpha x} \frac{\partial y(x)}{\partial y(0)} \tag{32}$$

where we have used the fact that $\beta q^2 \epsilon^{-1}(x) - 1 \approx \text{const} > 0$ for $T < T_c$. This integral will certainly be finite except possibly at $T = T_c$, in which case we want the asymptotic form of $y(x)$ as given by equation (29), since it is clear that $\partial y(x)/\partial y(0)$ is singular only at infinity.

Differentiating equation (21) with respect to $\tilde{y}(0)$ and using equation (29) we obtain

$$\frac{\partial}{\partial \tilde{x}} \left(\frac{\partial \tilde{y}(\tilde{x})}{\partial \tilde{y}(0)} \right) \underset{x\to\infty}{\sim} \frac{\partial \tilde{y}(\tilde{x})}{\partial \tilde{y}(0)} \frac{\ln \tilde{x}}{\tilde{x}} \tag{33}$$

which has the solution

$$\frac{\partial \tilde{y}(\tilde{x})}{\partial \tilde{y}(0)} \underset{x\to\infty}{\sim} \exp\{\tfrac{1}{2}(\ln \tilde{x})^2\}. \tag{34}$$

The integrals of the form (32) in the expression for C are thus all finite since the $e^{-\alpha x}$ factor ensures convergence. We can similarly show that all derivatives of C of finite order are finite and bounded at the critical temperature, which strongly indicates that C is analytic there.

It must be borne in mind that mean field approximations are notoriously bad in predicting the form of the singularities in specific heats etc, since such a theory ignores fluctuations in the internal field. We therefore expect that our value of T_c is an overestimate and that in an exact treatment there may be a weak singularity in C.

Just above the critical temperature, the largest pairs will dissociate and be able to carry charge so that the medium will conduct. Assuming that the mobility of a free charge behaves smoothly at T_c, the behaviour of the DC conductivity as $T \to T_c$ from above will be determined by that of the density of dissociated pairs $\delta n(T)$. This number may be estimated by calculating the number of pairs whose separation is less than R, where R is defined by $y(R) = 0$. When the separation r increases so that $y(r) < 0$, the trajectory $y(x)$ ($x = \ln(r/r_0)$) falls off rapidly to minus infinity (see figure A1). We interpret this failure of the theory as the complete dissociation of such a pair. We find that R is given by (see Appendix)

$$\ln \frac{R}{r_0} \underset{T \to T_c^+}{\sim} \exp\left\{\left(\ln \frac{1}{T - T_c}\right)^{1/2}\right\}. \tag{35}$$

The density of pairs with separation less than R is

$$\begin{aligned} n(R) &\approx \frac{2\pi}{r_0^2} \int_{r_0}^{R} \frac{\mathrm{d}r}{r_0} \left(\frac{r}{r_0}\right)^{-(2\beta q^2/\epsilon(r) - 1)} \\ &\approx \frac{\pi}{r_0^2} \frac{1 - (R/r_0)^{-2(\beta q^2 - 1)}}{\beta q^2 - 1} \end{aligned} \tag{36}$$

where we have taken $\epsilon(r) \approx 1$ throughout the region of integration. This is justified here because $\{\beta q^2/\epsilon(r)\} - 1 \approx 1$ near T_c for all r. Thus, the density of dissociated pairs $\delta n(T)$ is given by

$$\ln \frac{\delta n(T)}{n} \underset{T \to T_c^+}{\sim} -\exp\left\{\left(\ln \frac{1}{T - T_c}\right)^{1/2}\right\} \tag{37}$$

where $2n$ is the total density of charges. Also

$$\frac{\mathrm{d}}{\mathrm{d}T} \ln \frac{\delta n(T)}{n} \underset{T \to T_c^+}{\sim} \frac{\exp\left([\ln\{1/(T - T_c)\}]^{1/2}\right)}{T - T_c} \tag{38}$$

so that

$$\frac{\delta n(T)}{n} \underset{T \to T_c^+}{\to} 0 \tag{39}$$

and

$$\frac{\mathrm{d}^r}{\mathrm{d}T^r} \frac{\delta n(T)}{n} \underset{T \to T_c^+}{\to} 0 \,. \tag{40}$$

Thus, the DC conductivity tends to zero with all derivatives zero as the critical temperature is approached from above.

To conclude this section on the model system, we would like to point out that the assumption of a very dilute system ($e^{-2\beta\mu} \ll 1$) is not necessarily valid in a real system. However, we expect that the qualitative arguments will go through even in such a case and the general form of the results will be unchanged. We can imagine increasing the cutoff r_0 to some value R_0 such that the energy of two charges a distance R_0 apart is $2\mu(R_0)$ where $\exp\{-2\mu(R_0)\beta\} \ll 1$. For charges further apart than R_0, we can use the theory as outlined previously. The boundary conditions given by equation (20) will be changed to

$$y(0) = \frac{2q^2}{k_B T \epsilon(R_0)} - 4 \tag{41}$$

with $\epsilon(R_0)$ an unknown function. The critical temperature and the dielectric constant will now be determined in terms of $\epsilon(R_0)$ and $\mu(R_0)$. To determine these two quantities, a more sophisticated treatment is required, but we expect that the behaviour of the dielectric constant and specific heat at the critical temperature will be unchanged.

3. The two-dimensional *xy* model

The two-dimensional xy model is a system of spins constrained to rotate in the plane of the lattice which, for simplicity, we take to be a simple square lattice with spacing $\boldsymbol{a}$. The hamiltonian of the system is

$$H = -J \sum_{\langle ij \rangle} \boldsymbol{S}_i . \boldsymbol{S}_j = -J \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j) \tag{42}$$

where $J > 0$ and the sum $\langle ij \rangle$ over lattice sites is over nearest neighbours only. We have taken $|\boldsymbol{S}_i| = 1$ and ϕ_i is the angle the ith spin makes with some arbitrary axis. Only slowly varying configurations, that is, those with adjacent angles nearly equal, will give any significant contribution to the partition function so that may expand the hamiltonian up to terms quadratic in the angles.

It has been shown by many authors (Mermin and Wagner 1966, Wegner 1967, Berezinskii 1970) that this system does not have any long-range order as the ground state is unstable against low-energy spin-wave excitations. However, there is some evidence (Stanley 1968, Moore 1969) that this system has a phase transition, but it cannot be of the usual type with finite mean magnetization below T_c. As we shall show, there exist metastable states corresponding to vortices which are closely bound in pairs below some critical temperature, while above this they become free. The transition is characterized by a sudden change in the response to an applied magnetic field.

Expanding about a local minimum of H

$$H - E_0 \approx \tfrac{1}{2} J \sum_{\langle ij \rangle} (\phi_i - \phi_j)^2 = J \sum_{\boldsymbol{r}} (\Delta\phi(\boldsymbol{r}))^2 \tag{43}$$

where Δ denotes the first difference operator, $\phi(\boldsymbol{r})$ is a function defined over the lattice sites, and the sum is taken over all the sites. If we consider the system in the configuration of figure 1, its energy is, from equation (43)

$$H - E_0 \approx \pi J \ln \frac{R}{a} \tag{44}$$

where R is the radius of the system. Thus we have a slowly varying configuration, which we shall call a vortex, whose energy increases logarithmically with the size of the system.

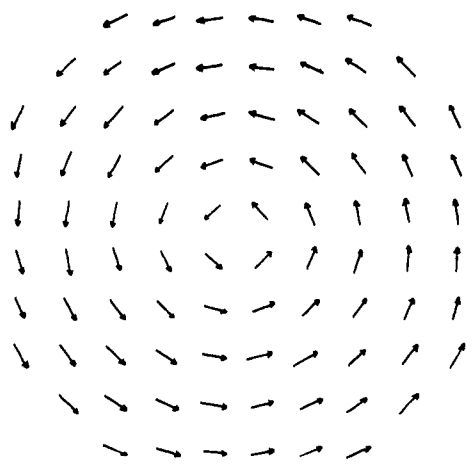

Figure 1. An isolated vortex in the xy model.

From the arguments of the Introduction, this suggests that a suitable description of the system is to approximate the hamiltonian by terms quadratic in $\Delta\phi(r)$ and split this up into a term corresponding to the vortices and another to the low-energy excitations (spin waves).

We extend the domain of $\phi(r)$ to $-\infty < \phi(r) < \infty$ to allow for the fact that, in the absence of vortices, $\langle(\phi(r) - \phi(r'))^2\rangle$ increases like $\ln(|r - r'|)$ (Berenzinskii 1971). Thus, at large separations, the spins will have gone through several revolutions relative to one another. If we now consider a vortex configuration of the type of figure 1, as we go round some closed path containing the centre of the vortex, $\phi(r)$ will change by 2π for each revolution. Thus, for a configuration with no vortices, the function $\phi(r)$ will be single-valued, while for one with vortices it will be many-valued. This may be summarized by

$$\overline{\sum} \Delta\phi(r) = 2\pi q \qquad q = 0, \pm 1, \pm 2 \ldots \tag{45}$$

where the sum is over some closed contour on the lattice and the number q defines the total strength of the vortex distribution contained in the contour. If a single vortex of the type shown in figure 1 is contained in the contour, then $q = 1$.

Let now $\phi(r) = \psi(r) + \bar{\phi}(r)$, where $\bar{\phi}(r)$ defines the angular distribution of the spins in the configuration of the local minimum, and $\psi(r)$ the deviation from this. The energy of the system is now

$$H - E_0 \approx J \sum_r (\Delta\psi(r))^2 + J \sum_r (\Delta\bar{\phi}(r))^2 \tag{46}$$

where

$$\overline{\sum} \Delta\psi(r) = 0 \qquad \text{and} \qquad \overline{\sum} \Delta\bar{\phi}(r) = 2\pi q. \tag{47}$$

The cross term vanishes because of the condition (47) obeyed by $\psi(r)$. Clearly the configuration of absolute minimum energy corresponds to $q = 0$ for every possible contour when $\bar{\phi}(r)$ is the same for all lattice sites. We see from equation (45) that, if we shrink the contour so that it passes through only four sites as in figure 2, we will obtain the strength

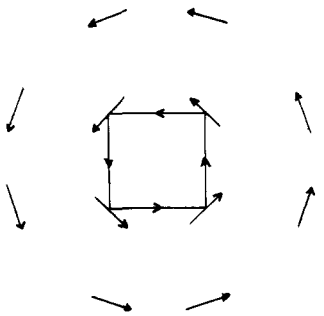

Figure 2. Contour around centre of vortex.

of the vortex whose centre we can take to be located on a dual lattice whose sites $\boldsymbol{r}^*$ lie at the centres of the squares of the original lattice (Berezinskii 1971). This procedure enables us to define the vortex distribution function $\rho(\boldsymbol{r}^*)$ given by

$$\rho(\boldsymbol{r}^*) = \sum_e q_e \, \delta_{\boldsymbol{r}^*\boldsymbol{r}_e^*} . \tag{48}$$

Going now to a continuum notation for convenience, using equation (47), we can easily find the equation obeyed by $\bar{\phi}(\boldsymbol{r})$

$$\nabla^2 \bar{\phi}(\boldsymbol{r}) = 2\pi\rho(\boldsymbol{r}). \tag{49}$$

In terms of ρ, the energy of the system in a given configuration is

$$H - E_0 = J \int \mathrm{d}^2\boldsymbol{r} (\nabla\psi)^2 - 4\pi^2 J \int\int \mathrm{d}^2\boldsymbol{r}\, \mathrm{d}^2\boldsymbol{r}'\, \rho(\boldsymbol{r})\, g(\boldsymbol{r} - \boldsymbol{r}')\, \rho(\boldsymbol{r}')$$
$$+ 2\pi J \int\int \mathrm{d}^2\boldsymbol{r}\, \mathrm{d}^2\boldsymbol{r}'\, \rho(\boldsymbol{r})\, \rho(\boldsymbol{r}') \ln \frac{R}{r_0} \tag{50}$$

where R is the radius of the system, r_0 is a cutoff of the order of the lattice spacing a and $g(\boldsymbol{r})$ is the Green function of the square lattice defined so that $g(0) = 0$ (Spitzer 1964). The last term of equation (50) requires that $\Sigma q_e = 0$ which is the condition that the total vorticity of the system vanishes, and corresponds to the requirement of electrical neutrality in the model system. The first term produces the spin-wave excitations and is responsible for destroying long-range order, and the second term is the interaction energy of the vortices which cause the phase transition.

If we ignore all vortex configurations, we obtain for the spin–spin correlation function

$$\langle \boldsymbol{S}_i . \boldsymbol{S}_j \rangle = \langle \exp\{\mathrm{i}(\phi_i - \phi_j)\} \rangle = \exp\left(- \frac{k_\mathrm{B} T}{2J} g(r_i - r_j) \right) \tag{51}$$

where (Spitzer 1964)

$$g(r) \underset{|r| \gg a}{\approx} \frac{1}{2\pi} \ln \left| \frac{r}{r_0} \right| \tag{52}$$

and

$$\frac{r_0}{a} = \frac{\mathrm{e}^{-\gamma}}{2\sqrt{2}} \qquad (\gamma = \text{Euler's constant}).$$

Thus

$$\langle \boldsymbol{S}_i \boldsymbol{S}_j \rangle \underset{|\boldsymbol{r}_i - \boldsymbol{r}_j| \gg a}{\approx} \left| \frac{\boldsymbol{r}_i - \boldsymbol{r}_j}{r_0} \right|^{-k_B T/4\pi J} \tag{53}$$

and we can see that the spin-wave excitations are responsible for destroying any long-range order in the system, but have nothing to do with any phase transition which may occur.

The energy E_v of the vortex configuration is now simply

$$E_v \underset{|\boldsymbol{r}_i - \boldsymbol{r}_j| \gg a}{\approx} - 2\pi J \sum_{i \neq j} q_i q_j \ln \left| \frac{\boldsymbol{r}_i - \boldsymbol{r}_j}{r_0} \right| \tag{54}$$

where q_i is the strength of the ith vortex whose centre is located at $\boldsymbol{r}_i$. We no longer distinguish between the original and dual lattices. This asymptotic expression for the energy is in fact a very good estimate even down to $|\boldsymbol{r}| = a$ (Spitzer 1964) so we can use it for all $|\boldsymbol{r}| > a$. Since in our approximation, the spin-waves and vortices do not interact with one another, the problem is now reduced to that of the model system with the vortices playing the rôle of the charged particles and

$$\begin{aligned} E_v &= - 2\pi J \sum_{i \neq j} q_i q_j \ln \left| \frac{\boldsymbol{r}_i - \boldsymbol{r}_j}{a} \right| - 2\pi J \sum_i q_i^2 \ln \frac{r_0}{a} && \text{for } |\boldsymbol{r}_i - \boldsymbol{r}_j| > a \\ &= 0 && \text{otherwise.} \end{aligned} \tag{55}$$

The chemical potential μ of a single vortex of unit strength is

$$\mu = - 2\pi J \ln \frac{r_0}{a} = 2\pi J(\gamma + \tfrac{3}{2} \ln 2) \tag{56}$$

which is to be compared with the exact expression for the energy of two vortices separated by a single lattice spacing

$$\mu = \pi^2 J \tag{57}$$

which is obtained from equation (50) using the exact value of $g(a) = \frac{1}{4}$. The critical temperature T_c at which the transition takes place is given by the solution of the equation

$$\begin{aligned} \frac{\pi J}{k_B T_c} - 1 &\approx \pi \tilde{y}_c(0) \exp\left(\frac{-\pi^2 J}{k_B T_c} \right) \\ &\approx 0{\cdot}12 . \end{aligned} \tag{58}$$

Below T_c, the vortices will be bound in pairs of zero total vorticity, while above T_c they are free to move to the surface under the influence of an arbitrarily weak applied magnetic field, thereby causing a sudden change in the form of the response to the applied field.

One way of seeing the effect of the transition is to consider the spin–spin correlation function $\langle \boldsymbol{S}_i . \boldsymbol{S}_j \rangle$. Taking the vortices into account, this is modified to

$$\langle \boldsymbol{S}_i . \boldsymbol{S}_j \rangle = \langle \exp\{\mathrm{i}(\psi_i - \psi_j)\} \rangle \langle \exp\{\mathrm{i}(\bar{\phi}_i - \bar{\phi}_j)\} \rangle . \tag{59}$$

Since the vortices and spin waves do not interact in our approximation, the two averages are taken independently. The average $\langle \exp\{\mathrm{i}(\psi_i - \psi_j)\} \rangle$ is taken over all possible values of ψ_i, and is given by equation (53) and $\langle \exp\{\mathrm{i}(\bar{\phi}_i - \bar{\phi}_j)\} \rangle$ is taken over all possible vortex distributions. In our mean field approximation, we can estimate the latter term as follows

$$\langle \exp\{\mathrm{i}(\bar{\phi}_i - \bar{\phi}_j)\} \rangle = \langle \bar{\boldsymbol{S}}_i . \bar{\boldsymbol{S}}_j \rangle \underset{|\boldsymbol{r}_i - \boldsymbol{r}_j| \to \infty}{\equiv} K(T) \tag{60}$$

where $\bar{S}_i$ is the spin on the ith site in the absence of spin-wave excitations. Thus,

$$K(T) = \bar{\sigma}^2 \tag{61}$$

where $\bar{\sigma}$ is the mean magnetization of the metastable configurations without the spin-wave excitations. Thus, $\bar{\sigma}$ corresponds exactly to ϵ^{-1} of the model system so that $K(T) = O(1)$ for $T < T_c$ and vanishes discontinuously at $T = T_c$ according to equation (27).

Since the spin waves and vortices do not interact, the system of vortices alone is equivalent to a system of freely moving, straight parallel current-carrying wires whose number is not conserved, located at the centres of the vortices. The sign of the forces between the wires is reversed, and $I_i = q_i\sqrt{2}\pi J$, I_i being the current in the ith wire in suitable units. The chemical potential $\mu = \pi^2 J$ is the energy required to 'create' a wire with no current. The sum of the currents in the wires is contained to be zero, corresponding to the condition $\Sigma q_i = 0$. This analogy tells us that, on applying a magnetic field in the plane of the system, the vortices will tend to move at right angles to the field, the direction determined by the sign of q_i.

4. Two-dimensional crystal

For simplicity, we consider a crystal with a square lattice of spacing a, and when possible as a continuum with a short distance cutoff r_0 of the order of the lattice spacing a. As far as any critical phenomena are concerned, this will make no essential difference. The short-distance behaviour will affect quantities like the effective chemical potential, but for our purposes we require only that this is sufficiently large. We can therefore use standard linear elasticity theory to describe our crystal (Landau and Lifshitz 1959).

The stress σ_{ij} is related to the strain u_{ij} for an isotropic medium by

$$\sigma_{ij} = 2\nu u_{ij} + \lambda\delta_{ij}u_{kk} \tag{62}$$

and the internal energy by

$$U = \tfrac{1}{2}\int \mathrm{d}^2\boldsymbol{r}u_{ij}\sigma_{ij}\,. \tag{63}$$

As mentioned in the Introduction, there is no long-range order of the usual type in this system, exactly as for the xy model of the previous section. Writing the energy in terms of the displacement field $\boldsymbol{u}(\boldsymbol{r})$, which describes the displacement of the lattice sites from their equilibrium positions, and expanding to terms quadratic in $\boldsymbol{u}(\boldsymbol{r})$, we can show that the mean square deviation of a site from its equilibrium position increases logarithmically with the size of the system (Peierls 1935, Berezinskii 1970). This destruction of long-range order is caused by the low-energy phonon modes, and the phase transition from the solid to the liquid state by the dislocation configurations. Since in our approximation, the phonons and dislocations do not interact, we may treat them separately. As in the magnetic case, we may decompose the displacement field as

$$\boldsymbol{u}(\boldsymbol{r}) = \boldsymbol{v}(\boldsymbol{r}) + \bar{\boldsymbol{u}}(\boldsymbol{r}) \tag{64}$$

where

$$\oint \boldsymbol{v}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{l} = 0 \qquad \text{and} \qquad \oint \bar{\boldsymbol{u}}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{l} = \boldsymbol{b} \tag{65}$$

where the integral is taken round some closed contour and $\boldsymbol{b}$ is the total Burger's vector of the dislocation distribution contained within the contour. $\boldsymbol{v}(\boldsymbol{r})$ is the displacement field of the phonons and $\bar{\boldsymbol{u}}(\boldsymbol{r})$ that of the dislocations. If the contour in equation (65) is taken round only one dislocation it gives the Burger's vector $\boldsymbol{b}$ of that dislocation. For simplicity we shall assume that $|\boldsymbol{b}|$ is the same for all dislocations and the most likely value of $|\boldsymbol{b}|$ will be the smallest possible, that is $|\boldsymbol{b}| \approx a$.

The most convenient way of treating a medium with dislocations is to introduce a stress function $\chi(\boldsymbol{r})$ which is related to the stress $\sigma_{ij}(\boldsymbol{r})$ by (Friedel 1964, Landau and Lifshitz 1959)

$$\sigma_{ij}(r) = \epsilon_{ik}\epsilon_{jl}\frac{\partial^2\chi(\boldsymbol{r})}{\partial x_k \partial x_l} \tag{66}$$

where

$$\epsilon_{12} = +1, \qquad \epsilon_{21} = -1, \qquad \epsilon_{ij} = 0 \text{ otherwise}.$$

We can then define a source function $\eta(\boldsymbol{r})$ describing the distribution of dislocations so that $\chi(\boldsymbol{r})$ obeys the equation

$$\nabla^4\chi(\boldsymbol{r}) = K\eta(\boldsymbol{r}) \tag{67}$$

where

$$K = \frac{4\nu(\nu + \lambda)}{2\nu + \lambda} = 2\nu(1 + \tau). \tag{68}$$

$\eta(\boldsymbol{r})$ is given by (Friedel 1964)

$$\eta(\boldsymbol{r}) = \sum_\alpha \epsilon_{ij} b_j^{(\alpha)} \frac{\partial}{\partial x_i^{(\alpha)}} \delta^{(2)}(\boldsymbol{r} - \boldsymbol{r}^{(\alpha)}) \tag{69}$$

where $\boldsymbol{r}^{(\alpha)}$ and $\boldsymbol{b}^{(\alpha)}$ are the position and Burger's vector respectively of the αth dislocation.

Having set up such a formalism, we can investigate the response of a medium containing dislocations to an applied stress in exact analogy to the electrostatic case. In our case, σ_{ij} and u_{ij} correspond respectively to the electric field $\boldsymbol{E}$ and displacement field $\boldsymbol{D}$. The strain energy of the medium due to the dislocations is

$$\begin{aligned} U &= \tfrac{1}{2}\int \mathrm{d}^2\boldsymbol{r}\, \chi(\boldsymbol{r})\,\eta(\boldsymbol{r}) \\ &= \frac{1}{2}K\int \mathrm{d}^2\boldsymbol{r}\, \mathrm{d}^2\boldsymbol{r}'\, \eta(\boldsymbol{r})\, g(\boldsymbol{r} - \boldsymbol{r}')\,\eta(\boldsymbol{r}') + \mathrm{O}\left(\sum_{\alpha\beta} \boldsymbol{b}^{(\alpha)} \cdot \boldsymbol{b}^{(\beta)} \ln\frac{R}{a}\right) \end{aligned} \tag{70}$$

where $g(\boldsymbol{r})$ is the Green function of equation (67)

$$g(\boldsymbol{r}) \underset{|\boldsymbol{r}| \gg a}{\approx} \frac{1}{8\pi}\boldsymbol{r}^2 \ln\left|\frac{\boldsymbol{r}}{\boldsymbol{r}_0}\right| \tag{71}$$

and

$$g(0) = 0.$$

Using those equations, we can immediately see that the energy of an isolated dislocation increases logarithmically with the area of the system. The strain energy of a pair of dislocations with equal but oppositely directed Burger's vectors is easily found to be (Friedel 1964)

$$U_{\text{pair}}(r) \underset{|\boldsymbol{r}| \gg a}{\approx} \frac{Kb^2}{4\pi}\left(\ln\left|\frac{\boldsymbol{r}}{a}\right| - \tfrac{1}{2}\cos 2\theta\right) + 2\mu \tag{72}$$

where $|r|$ is the separation of the two dislocations, θ the angle between $\boldsymbol{b}$ and $\boldsymbol{r}$, and 2μ the energy required to create two dislocations one lattice spacing apart. This result implies that, at low temperatures, the dislocations tend to form closely bound dipole pairs. Clearly, the condition $\Sigma \boldsymbol{b}^{(\alpha)} = 0$ must be satisfied so that at low temperatures the energy of the system is finite, corresponding to the condition of electrical neutrality in the model system.

The next step is to identify a quantity analogous to the dielectric constant. Consider the stress function $\chi^{(\alpha)}(\boldsymbol{r})$ due to the αth dipole with source function $\eta^{(\alpha)}(r)$, (cf Jackson 1962)

$$\chi^{(\alpha)}(\boldsymbol{r}) = K \int \mathrm{d}^2\boldsymbol{r}'\, \eta^{(\alpha)}(\boldsymbol{r}')\, g(\boldsymbol{r} - \boldsymbol{r}^{(\alpha)} - \boldsymbol{r}') \tag{73}$$

where $\boldsymbol{r}^{(\alpha)}$ denotes the centre of the αth dipole. Assuming the dipoles are very small, we expand in powers of $\boldsymbol{r}'$ for $|\boldsymbol{r}'| \ll |\boldsymbol{r} - \boldsymbol{r}^{(\alpha)}|$

$$\chi^{(\alpha)}(\boldsymbol{r}) = K \int \mathrm{d}^2\boldsymbol{r}'\, \eta^{(\alpha)}(\boldsymbol{r}')\, g(\boldsymbol{r} - \boldsymbol{r}^{(\alpha)}) + \tfrac{1}{2}K \int \mathrm{d}^2\boldsymbol{r}'\, \eta^{(\alpha)}(\boldsymbol{r}')\, x_i' x_j' \frac{\partial^2 g(\boldsymbol{r} - \boldsymbol{r}^{(\alpha)})}{\partial x_i^{(\alpha)} \partial x_j^{(\alpha)}} + \ldots \tag{74}$$

since the linear term vanishes for a dipole. We can now define the macroscopic stress function by averaging over a region ΔA such that $\langle r^2 \rangle \ll \Delta A \ll A$, where $\langle r^2 \rangle$ is the mean square separation of the dipole and A is the area of the system.

$$\chi(\boldsymbol{r}) \approx K \int \mathrm{d}^2\boldsymbol{r}' \eta(\boldsymbol{r}') g(\boldsymbol{r} - \boldsymbol{r}') + K \int \mathrm{d}^2\boldsymbol{r}' C_{ij}(\boldsymbol{r}') \frac{\partial^2 g(\boldsymbol{r} - \boldsymbol{r}')}{\partial x_i' \partial x_j'} \tag{75}$$

where

$$\eta(r) = \Big\langle \sum_\alpha \int \mathrm{d}^2\boldsymbol{r}' \eta^{(\alpha)}(\boldsymbol{r}') \delta(\boldsymbol{r} - \boldsymbol{r}^{(\alpha)}) \Big\rangle_{\Delta A} n(\boldsymbol{r}) \tag{76}$$

and

$$C_{ij}(r) = \tfrac{1}{2} \Big\langle \sum_\alpha \int \mathrm{d}^2\boldsymbol{r}' \eta^{(\alpha)}(\boldsymbol{r}') x_i' x_j' \delta(\boldsymbol{r} - \boldsymbol{r}^{(\alpha)}) \Big\rangle_{\Delta A} n(\boldsymbol{r})$$

where $n(\boldsymbol{r})$ is the density of dipoles.

Simple tensor analysis shows that, for an isotropic medium, C_{ij} is given in terms of the applied stress σ_{ij} by

$$C_{ij} = \epsilon_{ik}\epsilon_{kl}(C_1 \sigma_{kl} + C_2 \delta_{kl} \sigma_{mm}) + \mathrm{O}(\sigma^2) \tag{77}$$

where C_1 and C_2 are to be determined by a model calculation. From equation (75), we find after an integration by parts

$$\chi(\boldsymbol{r}) = \frac{K}{1 - K(C_1 + C_2)} \int \mathrm{d}^2\boldsymbol{r}' \eta(\boldsymbol{r}') g(\boldsymbol{r} - \boldsymbol{r}'). \tag{78}$$

Thus, the effect of the dislocation pairs is to renormalize $K^{-1} \to K^{-1} - (C_1 + C_2)$, and we immediately see that the quantity corresponding to the dielectric constant $\epsilon(r)$ is $\epsilon(r) = 1 - K\{C_1(r) + C_2(r)\}$. Using simple linear response theory as in the model system, we obtain

$$\begin{aligned} C_1(r) &= -\tfrac{1}{4}\beta b^2 n \langle r^2 \rangle \\ C_2(r) &= \tfrac{1}{8}\beta b^2 n \langle r^2 \cos 2\theta \rangle \end{aligned} \tag{79}$$

where the averages are to be taken with Boltzmann factor $\exp\{-\beta U_{\text{eff}}(r)\}$ and

$$U_{\text{eff}}(r) = \frac{b^2 K}{4\pi\epsilon(r)}\left(\ln\left|\frac{r}{r_0}\right| - \tfrac{1}{2}\cos 2\theta\right) + 2\mu. \tag{80}$$

Provided we choose the cutoff r_0 sufficiently large so that our continuum approximation holds, and that μ is large enough, we only have to show that the average over θ does not change the analogy with the model system of § 2. We can easily show that equation (19) is modified to

$$\frac{\mathrm{d}y}{\mathrm{d}x} = -\pi^2 \mathrm{e}^{-2\beta\mu}(y+4)^2\left(1 - \frac{I_1(2+\frac{1}{2}y)}{2I_0(2+\frac{1}{2}y)}\right)\mathrm{e}^{-xy} \tag{81}$$

with

$$y(x) = \frac{\beta b^2}{4\pi K\epsilon(x)} - 4$$

and $I_\nu(z)$ is the νth-order modified Bessel function (Ambramowitz and Stegun 1965). Provided μ is sufficiently large, $y(x)$ is very small for all x, so that the Bessel functions occurring in equation (81) are essentially constant. Thus we can immediately apply all the results of § 2 to this case.

5. Neutral superfluid

The same type of argument can be applied to a neutral superfluid in two dimensions. All that is required is that Bose condensation should occur in small regions of the system, so that locally a condensate wavefunction can be defined. The argument of Hohenberg (1967) shows that the phase of the condensate wavefunction fluctuates over large distances so that the type of order defined by Penrose and Onsager (1956) cannot occur. If a condensate wavefunction can be defined in a local region, it should be possible to explore the variation of its phase from one region to a neighbouring region. The total vorticity within a region is found by the change of phase along the boundary, divided by 2π. Just as the energy of a vortex in the magnetic system or dislocation in the crystal, so the energy of a superfluid vortex increases logarithmically with the size of the system. At low temperatures, there will be no free vortices, only clusters of zero total vorticity. Neglecting the interaction between clusters, the critical temperature is given by equation (5). The analogy with the model system is close as there is only one type of vortex which may have either sign. As in this model, we expect the interaction between vortex clusters to lower the critical temperature from the estimate of equation (5). The lattice Bose gas has been discussed in detail by Berezinskii (1971) who finds the parameters of the Bose gas to be related to those of the magnetic system by

$$J = \frac{\rho\hbar^2}{m} \qquad \text{and} \qquad r_0 \approx 1{\cdot}28\frac{\hbar c}{T}$$

where c is the speed of sound. Using these parameters, we can estimate the value of T_c from equation (58) and the superfluid density $\rho_s(T_c)$ which is nonzero in contrast to the result of Berezinskii.

Below the critical temperature, for a lattice Bose system with periodic boundary conditions, superfluid flow is stable in the thermodynamic limit, since a state with flow is one in which the phase of the order parameter changes by a multiple of 2π round the

system. The system can change from one such state to another by the creation and separation of a pair of vortices, one of which passes right round the system before recombining with the other, but there is a high energy barrier which prevents this process. The different states of superfluid flow are topologically distinct states which do not make transitions between one another at low temperatures. The phase transition is characterized by these states becoming mutually accessible above the transition temperature, so that the flow states are no longer metastable.

Experiments on the onset of superfluid flow for thin films—see, for example, Symonds *et al* (1966), Chester *et al* (1972) and Herb and Dash (1972)—show a strong depression of the temperature as the film becomes thinner. According to the considerations of this paper the critical temperature should be given by

$$k_B T_c = \frac{\pi \hbar^2 \rho_s}{2m^*} \tag{82}$$

where ρ_s is the density of superfluid particles per unit area and m^* is the effective mass of the helium atoms in the film. If ρ_s is taken to be the bulk value multiplied by the film thickness and m^* is taken to be unaffected by the substrate, and so equal to the atomic mass, this formula gives too high a value for T_c, so the effect of the boundaries in reducing ρ_s must be important. The value of ρ_s at the onset temperature must be nonzero; for a film thickness 1·5 nm at 1·5 K the superfluid density given by equation (81) is about 0·22 times the particle density, if m^* is taken equal to the atomic mass. It is not surprising that the specific heat maximum occurs at a higher temperature than the onset of superfluidity, since a considerable degree of short-range order is necessary before the considerations of this paper have any relevance. De Gennes has made a relevant comment on this matter (see Symonds *et al* 1966).

For a charged superfluid (superconductor) the argument cannot be carried through because, as a result of the finite penetration depth λ, the energy of a single flux line is finite. The circulating current density inside a thin superconducting film of thickness $d \ll \lambda$ is (Pearl 1964)

$$\begin{aligned} J(r) &\approx \frac{\hbar c^2}{4e} \frac{d}{\lambda^2} \frac{1}{r} && r \ll \frac{\lambda^2}{d} \\ &\approx \frac{\hbar c^2}{4\pi e} \frac{1}{r^2} && r \gg \frac{\lambda^2}{d} \end{aligned} \tag{83}$$

where r is the distance from the flux line. The repulsion energy between two vortices with opposite circulation falls off like r^{-1} instead of increasing as $\ln r$ for large separations. The self energy of a single flux line is thus determined by the current near the flux line and is approximately (De Gennes 1966)

$$U \approx \left(\frac{\hbar c}{4e}\right)^2 \frac{d}{\lambda^2} \ln \frac{\lambda^2}{d\xi} \tag{84}$$

where ξ is the 'hard core' radius of the flux line.

6. Isotropic Heisenberg model in two dimensions

The isotropic Heisenberg model for a two-dimensional system of spins is quite different from the xy model. To show the nature of this difference, we consider a large system

with periodic boundary conditions, but similar considerations apply to other boundary conditions. In the xy model at low temperatures, the direction of magnetization in a region is defined by a single angle ϕ which varies slowly in space. Although the angle ϕ fluctuates by a large amount in a large system, the number of multiples of 2π it changes by on a path that goes completely round the system is a topological invariant, so that

$$n_x = \frac{1}{2\pi}\int_0^{L_x} \frac{\partial \phi}{\partial x}\,\mathrm{d}x \qquad n_y = \frac{1}{2\pi}\int_0^{L_y} \frac{\partial \phi}{\partial y}\,\mathrm{d}y \tag{85}$$

are numbers defining a particular metastable state. Transitions can only take place from one metastable state to another if a vortex pair is formed, the two vortices separate and recombine after one has gone right round the system. Such a process will cause a change of one in either n_x or n_y, but there is a logarithmically large energy barrier to prevent such a transition.

In the case of the isotropic Heisenberg model, the direction of magnetization is defined by two polar angles θ and ϕ. A quantity such as

$$\frac{1}{2\pi}\int_0^{L_x} \frac{\partial \phi}{\partial x}\mathrm{d}x$$

is not a topological invariant. A twist of the angle ϕ by 2π across the system can be changed continuously into no twist by changing the other polar angle θ (which we take to be the same everywhere) from $\frac{1}{2}\pi$ to zero. There is in fact a single topological invariant for the Heisenberg model in two dimensions, which is

$$N = \frac{1}{4\pi}\int\int \sin\theta\left(\frac{\partial\theta}{\partial x}\frac{\partial\phi}{\partial y} - \frac{\partial\theta}{\partial y}\frac{\partial\phi}{\partial x}\right)\mathrm{d}x\,\mathrm{d}y. \tag{86}$$

If we regard the direction of magnetization in space as giving a mapping of the space on to the surface of a unit sphere, this invariant measures the number of times the map of the space encloses the sphere. This invariant is of no significance in statistical mechanics, because the energy barrier separating configurations with different values of N is of order unity. To show this, we consider how a configuration with N equal to unity can be transformed continuously into one with N equal to zero.

A simple example of a configuration with $N = 1$ is one in which θ is a continuous function of $r = (x^2 + y^2)^{1/2}$, equal to π for r greater than some value a, and equal to zero at the origin. The angle ϕ is assumed to be equal to $\tan^{-1}(y/x)$. The energy of a slowly varying configuration is proportional to

$$\tfrac{1}{2}\int\int ((\nabla\theta)^2 + \sin^2\theta(\nabla\phi)^2)\,\mathrm{d}x\,\mathrm{d}y$$

which, for the configuration described above

$$= \pi\int_0^a \left\{\left(\frac{\mathrm{d}\theta}{\mathrm{d}r}\right)^2 + \frac{1}{r^2}\sin^2\theta\right\} r\,\mathrm{d}r. \tag{87}$$

Even if θ varies linearly between the origin and $r = a$, this integral is finite and independent of a. The configuration can be changed continuously into a configuration with $N = 0$ by letting a tend to zero. Of course, for small values of a, this expression for the energy is invalid, but the number of spins in a disc of radius a is then small so that any energy barrier is small.

We must conclude that there is no topological long-range order in the Heisenberg model in two dimensions. Supposing that the occurrence of a phase transition is really connected with the existence of long-range order we would conjecture that the xy model has a phase transition but the Heisenberg model does not. Such a conjecture does not seem to be in conflict with the evidence provided by the analysis of power series for the models by Stanley (1968) and Moore (1969).

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Appendix. Solution of $dy/dx = -e^{-xy}$

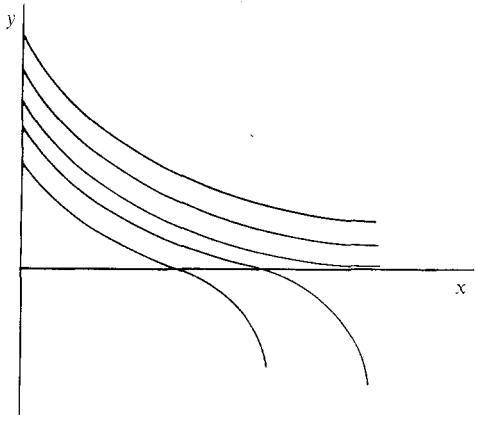

Figure A1. Trajectories of $dy/dx = e^{-xy}$.

From the method of isoclines, we see that the trajectories $y(x)$ behave as plotted in figure A1 with the singular point at infinity. It is easy to see that the solutions fall into two classes

$$\begin{aligned} &\text{(i)} \qquad y(\infty) \geqslant 0 \qquad\qquad y(0) \geqslant y_c(0) \\ &\text{(ii)} \qquad y(\infty) \to -\infty \qquad y(0) < y_c(0) \end{aligned} \tag{A.1}$$

corresponding to equation (22). For convenience, we make a transformation of variables to brong the singular point to the origin by defining

$$z = \frac{1}{xy} \qquad w = xy - \ln\frac{x}{y} \tag{A.2}$$

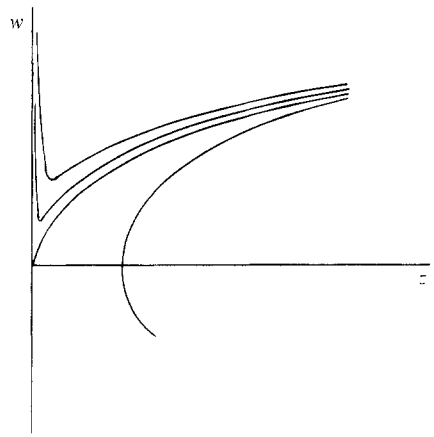

Figure A2. Trajectories in transformed variables.

so that

$$\frac{dw}{dz} = -\frac{1}{z^2} + \frac{1}{z}\coth \tfrac{1}{2}w. \tag{A.3}$$

The trajectories $w(z)$ have the form displayed in figure A2, where the trajectories corresponding to $y(0) \geqslant y_c(0)$ are those with $w(z) \geqslant 0$. We can find approximate solutions in the three regions

(i) $w \sim 0, \quad z \sim 0$

(ii) $w \to \infty, \quad z \sim 0$

(iii) $w \to \infty, \quad z \to \infty$

and match the solutions at $w = 2$. In region (i)

$$\frac{dw}{dz} \approx -\frac{1}{z^2} + \frac{2}{wz}\,. \tag{A.4}$$

Changing variables to $2t = (1/z) - w$ we obtain

$$z(t) \approx e^{t^2} \int_t^{t_1} e^{-s^2}\, ds \tag{A.5}$$

where $t_1 \to \infty$ as $y(0) \to y_c(0)$ from above. In regions (ii) and (iii)

$$w(z) \approx \frac{1}{z} + \ln z + 2 \ln y \tag{A.6}$$

where $y = y(\infty)$ in (ii) and $y = y(0)$ in (iii).

We can make the best match at $w(z) = 2$, where the gradients in the three regions are equal. However, the numbers are not too good because $\coth 1 \approx \frac{2}{3}$, while we have taken $\coth \frac{1}{2}w = 1$ in regions (ii) and (iii). The points at which we match are defined by the intersections of the curves

$$z(t) = \frac{1}{2(t+1)} \qquad \text{and} \qquad z(t) = e^{t^2} \int_t^{t_1} e^{-s^2}\, ds. \tag{A.7}$$

The match between regions (i) and (ii) corresponds to the intersection at $t \to \infty$, that is

$$t \approx t_1 - \frac{\ln t_1}{2t_1}. \tag{A.8}$$

At the other intersection, we put $t = t_c + \delta$, where t_c is defined by

$$z_c(t_c) = \frac{1}{2(t_c + 1)} = e^{t_c^2} \int_{t_c}^{\infty} e^{-s^2}\, ds. \tag{A.9}$$

Numerical calculations give $t_c \approx -0{\cdot}84$. Expanding $z(t)$ to first order in δ we obtain

$$t \approx t_c + \frac{(t_c + 1)\, e^{t_c^2}}{(-2t_c - 1)} \frac{e^{-t_1^2}}{t_1}. \tag{A.10}$$

Using equations (A.6) to (A.10), we obtain

$$\begin{aligned} y(\infty) &\approx \sqrt{2} t_1\, e^{-t_1^2} \\ y(0) - y_c(0) &\approx \frac{(1 + t_c)^2 \exp(t_c^2 - 2t_c)}{2y_c(0)} \frac{e^{-t_1^2}}{t_1} \end{aligned} \tag{A.11}$$

where

$$y_c^2(0) = 2(t_c + 1)\, e^{-2t_c} \approx 1{\cdot}7. \tag{A.12}$$

Taking logarithms of equation (A.11) eliminating t_1, we obtain the leading singularity in $y(\infty)$ for $y(0) \gtrsim y_c(0)$

$$\ln y(\infty) \sim -\left(\ln \frac{1}{y(0) - y_c(0)}\right)^{1/2}. \tag{A.13}$$

Substituting the expressions for $y(\infty)$ and $y(0)$ given by equation (20), and ignoring all but the most singular terms, we immediately obtain equation (27).

Just above the critical temperature where $y(0) \leqslant y_c(0)$, the appropriate solution of equation (A.4) is

$$z(t) = e^{t^2} \int_t^{\infty} e^{-s^2}\, ds + K e^{t^2} \tag{A.14}$$

where $K \geqslant 0$. In the region $w \to -\infty, z \to +\infty$

$$w(z) \approx \frac{1}{z} - \ln z - 2 \ln X \tag{A.15}$$

where X is defined by $y(X) = 0$. We can now carry out exactly the same procedure as above to estimate the behaviour of X for $y(0) \to y_c(0)$ when $K \to 0^+$ by matching the solutions (A.6), (A.14) and (A.15) at $w = \pm 2$. We find

$$\ln X \underset{y(0) \to y_c(0)}{\sim} \{-\ln(y_c(0) - y(0))\}^{1/2}. \tag{A.16}$$

Using the expressions for $y(0)$ and $y_c(0)$ of equation (20), we immediately obtain equation (35).

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