SUPERFLUIDITY, MELTING AND LIQUID-CRYSTAL PHASES IN TWO DIMENSIONS

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Contents

1. INTRODUCTION

Phase transitions in two-dimensional systems are interesting to the theorist for a number of reasons. In general, long wavelength fluctuations are more important in two dimensions than in three dimensions, and deviations from the mean-field theory are much greater. In two-dimensional systems with a continous symmetry group, one commonly finds that there is a divergence in the fluctuations of the phase of the order parameter in the low temperature state, arising from the effects of long-wavelength excitations. This divergence causes the mean value of the order parameter to vanish,[1] so that the low temparature phase cannot be characterized by a true long range order,or broken symmetry, in the two-dimensional case, as it can in the three-dimensional counterparts.

In some cases (e.g., the two-dimensional Heisenberg model), long wavelength fluctuations apparently eliminate the phase transition altogether.[2] In the systems that will be discussed in the present series of lectures, however, there is still a kind of quasi-long-range order in the low temperature phase, characterized by a power-law decay of the order parameter correlation function.[3] This quasi-long range order is mathematically distinct from short-range order (exponental decay of the correlation function at large distances)which is expected at high temperatures, so there must be a mathematically well-defined transition temperature T_c separating the two types of behavior.

The general mathematical methods for studying this type of phase transition were developed by Kosterlitz and Thouless in the early 1970's.[4-7] In these lectures, I shall review the Kosterlitz-Thouless theory, and discuss some of the recent developments in the field. As in the Kosterlitz-Thouless theory, our attention will be focused on the behavior of topological defects such as vortices, dislocations or disclinations, which are responsible for the phase transitions, and the destruction of the quasi-long range order.[4,8]

In Section 2, below, I shall discuss with some care the relations between a superfluid and the planar-spin model or X-Y model of magnetism which was discussed in Prof. Suzuki's talk.[9] I shall discuss the role of vortices in destroying persistent currents in the superfluid, and in destroying the property of quasi-long range order when the phase transition occurs. I shall derive the formulae for the energy of a system of vortices and develop the analogy with Coulomb charges in two-dimensions.[4,8] The Kosterlitz recursion relations[5] will be derived and we shall review the results of this renormalization group theory.

In Section 3, I shall discuss the dynamics of the superfluid system, with and without vortices. Results of the static calculations of Sec. 2 will be used to calculate dynamic properties of a helium film near the superfluid transition temperature.[10-13]

In Section 4, I shall briefly discuss the effects of a symmetry-breaking perturbation proportional to cos $p\phi$, where ϕ is the phase of the order parameter, and p is an integer. This perturbation removes the continuous symmetry group present in the planar-spin model Hamiltonian discussed in Sec. 2. Nevertheless, under certain conditions, the phenomenon of quasi-long-range order may occur, and the phase transition to the high temperature paramagnetic state (short range order) may be identical to that in the continuous-symmetry planar spin model.[14]

In Section 5, I shall discuss the recent theory of melting in two dimensions, based on the assumption that the crystal is destroyed by a phase transition of the Kosterlitz-Thouless type, with dislocations taking the place of the vortices which occurred in the planar-spin model.[15-18] We shall see that there are many similarities between the melting transition and transition in the superfluid or planar-spin-model, discussed in Sec. 2, but there are also some interesting differences between the two cases.

In Section 6, I shall discuss the situation which occurs in smectic liquid-crystal layers, when the molecular axis is tilted relative to the normal to the layer. I shall describe briefly the different phases which may occur when one takes account of the coupling beyween the order parameter describing the orientation of the molecular axes and the various order parameters describing the location of the molecules within the plane.[19] The possible relevance of the two dimensional theories to bulk smectic phases will be mentioned.

Acknowledgments

In all those aspects of this subject to which I have made some contribution, my work has been done in collaboration with others. In particular, the dynamic theory which will be presented in section 3 below was developed in collaboration with V. Ambegaokar, D.R. Nelson, and E.D. Siggia. The work on the theory of melting, discussed in Sec. 5, and on the liquid crystal phases, discussed in Sec. 6, was done in collaboration with D.R. Nelson. I have learned a great deal from these collaborators.

My understanding of order in two-dimensional systems has also been shaped by conversations with many other colleagues, dating back as far as 1966. I can only mention here a few who have been most helpful to me in the subjects covered by these lectures: R. Morf, A. Zippelius, R. Pelcovits, R. Petschek, D. S. Fisher, P. C. Hohenberg, P. C. Martin, S. Hikami, R. Pindak, C. C. Grimes, R. J. Birgeneau, P. Pershan and A. P. Young.

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2. SUPERFLUIDITY AND THE PLANAR-SPIN MODEL

A. Long-range order and quasi-long-range order.

We consider here a model with a two component order parameter, $\vec{S} = (S_x, S_y)$, or in complex notation

$$\psi = S_x - iS_y . \tag{2.1}$$

The order parameter may be defined at a lattice of discrete points as in Professor Suzuki's talk,[9] but it will be more convenient for our purposes to define the order parameter as a continuous function of position $\vec{r}$. (A discrete model may always be converted to a continuous model by a suitable interpolation between the lattice sites.) In order to have the correct number of degrees of freedom for this system, we shall restrict the wave vector $\vec{k}$ to be less than a cutoff Λ, which is the order of the reciprocal of the lattice constant $\underline{a}$. We may assume for concreteness that the energy H has the Ginzburg-Landau form[20,21]

$$H = \int d^2r \; [- \frac{\alpha}{2} |\psi|^2 + \frac{\beta}{4} |\psi|^4 + \frac{J}{2} |\nabla\psi|^2 + \ldots], \tag{2.2}$$

which defines an equilibrium probability distribution for ψ, of the form[22]

$$P_{eq}[\psi] \propto e^{-H/T} . \tag{2.3}$$

For generality, we may assume that H has already included the effects of fluctuations in degrees of freedom other than ψ, or of fluctuations in ψ on a scale shorter than $1/\Lambda$, and therefore the coefficients α, β, and J will generally be (analytic) functions of temperature.

If we are interested in T = 0, we need only minimize H. We thus find

$$\psi(\vec{r}) = |\psi_0| e^{i\phi} , \qquad (2.4)$$

where ϕ is an arbitrary constant and

$$|\psi_0|^2 = \frac{\alpha}{\beta} . \qquad (2.5)$$

By symmetry, the energy H is independent of the value of the phase ϕ.

What happens at $T \neq 0$? In three dimensions, we may use the Landau theory, or the mean field theory, to get a reasonable approximation.[21] One then finds that there exists a transition temperature T_c, such that for all temperatures less than T_c,

$$\psi(\vec{r}) = M\, e^{i\phi} \neq 0 . \qquad (2.6)$$

Here, the magnetization M depends on temperature, whereas the phase ϕ is an arbitrary constant. Alternatively, we may define magnetization M through the long distance behavior of the correlation function

$$\lim_{r\to\infty} \langle \psi^*(\vec{r})\psi(0)\rangle = M^2 \neq 0 . \qquad (2.7)$$

When (2.7) applies, we say that there is long range order for the parameter ψ. Note that the phase factor $e^{i\phi}$ has dropped out of Eq. (2.7)

For all $T > T_c$ we have

$$\psi(\vec{r}) = 0 , \qquad (2.8)$$

$$\langle \psi^*(\vec{r})\psi(0)\rangle \sim e^{-r/\xi_+}, \quad \text{for } r\to\infty . \qquad (2.9)$$

In this case, we say that there is short range order for the parameter ψ. As T approaches T_c we find, in the Landau theory,

$$M \sim (T_c - T)^{1/2} , \qquad (2.10)$$

$$\xi_+ \sim (T-T_c)^{-1/2} \quad . \tag{2.11}$$

Although Landau theory is not correct at the transition temperature, the qualitative picture in three dimensions is reasonably good. When the effect of long wave length fluctuations are properly taken into account, the principal change is that the exponents ½ appearing in Eqs. (2.10) and (2.11) are replaced by quantities approximately equal to 1/3 and 2/3 respectively.[21,23]

In two dimensions, the effects of fluctuation are much more drastic. At low temperatures, we may as a first approximation neglect fluctuations in the magnitude $|\psi(\vec{r})|$. Let us write:

$$\psi(\vec{r}) = \psi_0 e^{i\phi(\vec{r})} \quad . \tag{2.12}$$

Then the energy is given by

$$H = \tfrac{1}{2}\int K_0 |\nabla\phi|^2 d^2r \quad , \tag{2.13}$$

$$K_0 \equiv J_0 |\psi_0|^2 \quad . \tag{2.14}$$

Since Eq. (2.13) is quadratic in ϕ, the variable ϕ has a Gaussian distribution, and we can easily calculate correlation function

$$\begin{aligned} \langle\psi^*(\vec{r})\psi(0)\rangle &= |\psi_0|^2 \langle e^{-i\phi(\vec{r})} e^{i\phi(0)}\rangle \\ &= |\psi_0|^2 \exp\{-\tfrac{1}{2}\langle[\phi(\vec{r})-\phi(0)]^2\rangle\} \quad . \end{aligned} \tag{2.15}$$

The last quantity can be evaluated using Fourier transforms, as discussed in Professor Suzuki's lecture:[9]

$$\langle[\phi(\vec{r}) - \phi(0)]^2\rangle = \int \frac{d^2k}{(2\pi)^2} \; |e^{i\vec{k}\cdot\vec{r}}-1|^2 \langle|\phi(\vec{k})|^2\rangle \quad . \tag{2.16}$$

The factor $|e^{i\vec{k}\cdot\vec{r}}-1|^2$ can be approximated by 2, its average value, in the interval $1/r<k<1/a$. Then, using the equipartition theorem we find

$$<[\phi(\vec{r})-\phi(0)]^2> = \frac{2}{(2\pi)^2} \int_{1/r}^{1/a} 2\pi k dk \left(\frac{T}{K_0 k^2}\right)$$

$$\approx \frac{T}{\pi K_0} \ln(r/a) \qquad (2.17)$$

Hence, for large r,[3]

$$<\psi^*(\vec{r})\psi(0)> \sim (1/r)^\eta \qquad (2.18)$$

where

$$\eta = \frac{T}{2\pi K_0} \quad . \qquad (2.19)$$

This power-law behavior is not true long range order as in (2.18), but it certainly differs from ordinary short range order, defined by exponential decay of correlations, as in (2.9). When (2.18) applies, we shall say that the order parameter ψ shows *quasi-long-range order*.

B. *Vortices*

What are the effects of magnitude fluctuation? Let us write:

$$\psi(\vec{r}) = |\psi(\vec{r})| e^{i\phi(\vec{r})} \quad . \qquad (2.20)$$

We shall assume that ψ is a continuous, differential function of position. If $\vec{r}$ is defined in a simply connected region S, and if $\psi(\vec{r}) \neq 0$ everywhere in this region, then it is possible to choose $\phi(\vec{r})$ to be continuous, differentiable and *single-valued*. On the other hand, if $\psi(\vec{r}) = 0$ at any point in the region, or if the region S is multiply-connected, then in general we must choose ϕ to be a *multiple-valued* function of position. The phase ϕ is then continuous and differentiable except at the set of points $\{\vec{R}_i\}$, where $\psi = 0$. [Alternatively, if one wished to employ a single value function ϕ, it would be necessary to introduce *lines* where ϕ is discontinuous by 2π.]

[Because $\psi(\vec{r})$ is a smoothly varying random function, one can show that with probability unity, ψ will vanish only at isolated points in the two-dimensional space. These points will be the intersections of the curves described by the equations Re $\psi = 0$, and Im $\psi = 0$.]

It is clear from the above that we must draw an important distinction between small fluctuations in the magnitude of ψ, such that ψ does not go to 0, and large fluctuations, where $\psi(\vec{r})$ can pass through 0. Although small fluctuations do lead to a renormalization of the elastic constant K as will be discussed below, they have few other effects and they have been shown to be "irrelevant" in a renormalization group sense, throughout the temperature range of interest.[24] We shall ignore small magnitude fluctuations in the remainder of these lectures. On the other hand, large magnitude fluctuations, points where $\psi(\vec{r}) = 0$, will play a very important role in our analysis.

In order to avoid the complications arising from the multivaluedness of ϕ, it is convenient to work with the gradient of ϕ, which is single valued. Let us define

$$\vec{v}(r) \equiv \vec{\nabla}\phi(\vec{r}) \quad . \tag{2.21}$$

Then for any closed contour C,

$$\begin{aligned}\oint_C \vec{v}(r)\cdot d\vec{r} &= \text{phase change along contour C} \\ &= 2\pi N \ ,\end{aligned} \tag{2.22}$$

where N is an integer, since $e^{i\phi}$ must be single-valued.

Let $\vec{R}_i$ be a point where $\psi = 0$. We say that there is a <u>vortex</u> at $\vec{R}_i$, and we define a vortex charge N_i, by

$$N_i \equiv \frac{1}{2\pi}\oint_{C_i} \vec{v}\cdot d\vec{r} \quad , \tag{2.23}$$

where C_i is a small contour just enclosing point $\vec{R}_i$. In actuality, only the cases $N_i = \pm 1$ need be considered. (Note: When applied to the planar spin model the vortex is often described as a <u>disclination</u> in the vector-field $\vec{S}$.)

For a general contour C,

$$\oint_C \vec{v}\cdot d\vec{r} = \sum_i{}' 2\pi N_i \equiv 2\pi N_C \tag{2.24}$$

where the prime on the summation indicates that we should sum over all vortices located inside the contour C. Let us define a vortex charge <u>density</u> by

$$N(\vec{r}) \equiv \sum_i N_i \delta(\vec{r}-\vec{R}_i) \quad . \qquad (2.25)$$

According to (2.24), we may write:

$$\vec{\nabla} \times \vec{v} = 2\pi N(\vec{r}) \quad . \qquad (2.26)$$

If $\psi(\vec{r})$ varies continuously in time, then in general the positions of the vortices R_i will also be continuous functions of the time t. Now, consider the integral on the left hand side of Eq. (2.24). If the function $\psi(\vec{r})$ does not vanish at any point on the contour C, then it is clear that v must be a continuous function of position and time, and the integral is a continuous function of t. But the right-hand side of (2.24) can only change discontinuously since N_i must be an integer. It follows that the net vortex charge enclosed by C cannot change at all, unless ψ vanishes at some point on the boundary C - that is, unless a vortex crosses the contour C.[25] Thus, for a general region S, the total vortex charge in the region can only change if a vortex enters or leaves the region at the boundary. Note that if a vortex is created or annihilated at an <u>interior</u> boundary of a multiply connected region, there will be an image charge left on the boundary and the net vorticity in the region is unchanged. [Of course, the total <u>number</u> of vortices (positive <u>plus</u> negative) can be changed by processes in which a pair of vortices of opposite sign is either created or annihilated in the interior of the region.] In any case, we have a conservation of vortex charge, and we may write:

$$\frac{\partial N}{\partial t} = -\vec{\nabla}\cdot\vec{J}_v \qquad (2.27)$$

where $\vec{J}_v$ is the <u>vortex current</u>

$$\vec{J}_v \equiv \sum_i N_i \frac{d\vec{R}_i}{dt} \delta(\vec{r}-\vec{R}) \quad . \qquad (2.28)$$

Let us now consider an elementary vortex at the origin with $N_i=\pm 1$. We wish to find the state of lowest energy. It is clear from symmetry that the phase ϕ should change in a uniform matter as one goes around a circle enclosing the origin. Therefore, we may write:

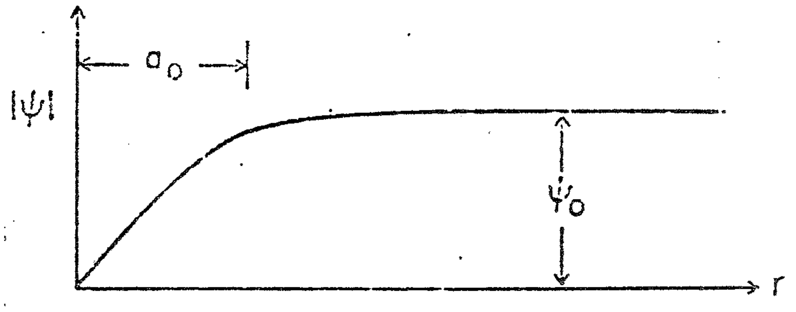
$$e^{i\phi(\vec{r})} = \frac{x \pm iy}{|r|} \cdot e^{i\phi_0} , \qquad (2.29)$$

where ϕ_0 is an arbitrary constant and the ± refers to $N_i = \pm 1$. In either case, we have

$$|\vec{\nabla}\phi| = 1/r . \qquad (2.30)$$

The magnitude of ψ is shown schematically in Fig. 1.[26]

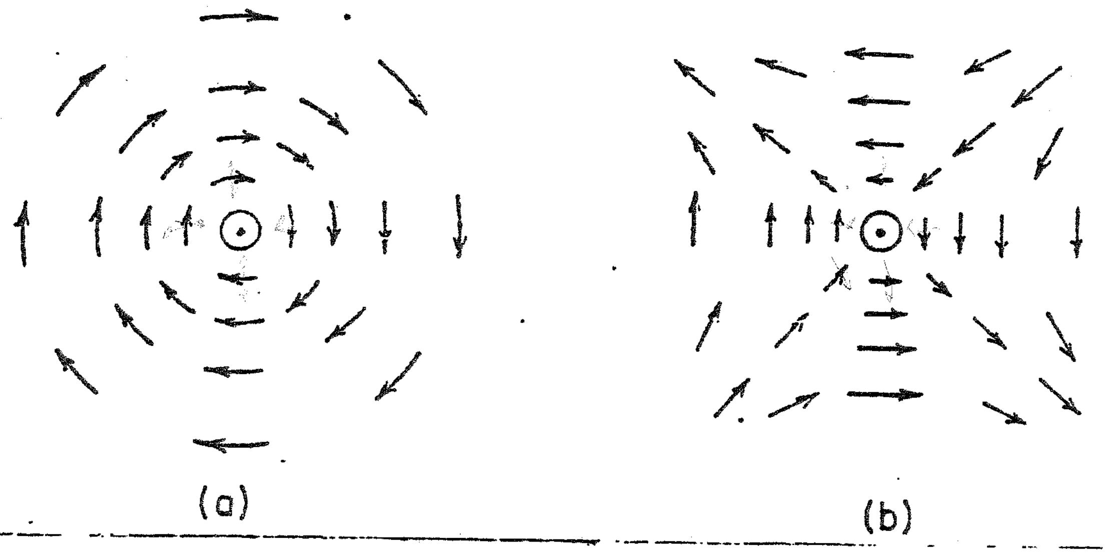
Fig. 1. Magnitude of the order parameter ψ as a function of distance from the center of a vortex.



Far from the origin, for $r \gg a_0$, the magnitude $|\psi|$ is approximately equal to its equilibrium value ψ_0, given in terms of the Ginzburg-Landau parameters by Eq. (2.5). The radius a_0 is given approximately by $a_0 = (\alpha/J)^{-\frac{1}{2}}$. Near the origin $|\psi(\vec{r})|$ rises linearly from 0 and

$$\psi(\vec{r}) = (x \pm iy)/a_0 \qquad (2.31)$$

Note that the real and imaginary parts of ψ are continuous and differentiable at the origin. The spin configurations for vortices with $N_i = \pm 1$ are illustrated in Fig. 2.



(a) (b)

Fig. 2. Spin configuration in the vicinity of a vortex. Arrows indicate orientation and magnitude of spin-vector $\vec{S}$*, and do not coincide with direction of* $\vec{v}_s$*. With our convention,* ($\psi = S_x - iS_y$)*, the vortices in (a) and (b) have charges* $N_i = -1$ *and* $N_i = 1$ *respectively. Note that reversing the directions of all arrows, or rotating them through a constant angle, is equivalent to multiplication of* ψ *by a constant phase-factor, and has no effect on* $\vec{v}_s$ *or* N_i

The energy H_1 of an isolated vortex may be readily estimated. For $r > a_0$, Eq. (2.13) may be used. We find that

$$H_1 = E_c + \int_{a_0}^{R} 2\pi r dr \cdot \frac{K_0}{2} |\nabla\phi|^2$$

$$= E_c + \pi K_0 \ln(R/a_0) \qquad (2.32)$$

where R is the radius of the system, and E_c is the core correction coming from regions where $r > a_0$. In the Ginzburg-Landau theory, E_c is equal to a constant times K_0, and K_0 is given by Eq. (2.14). Notice that energy of an isolated vortex tends to infinity if the radius of the system goes to infinity.[27]

This divergence may be eliminated if one considers a pair of vortices of opposite sign (see Fig. 3). Because of cancellation from the two vortices, the gradient $\vec{v}$ falls off faster than 1/r for distances large compared to the

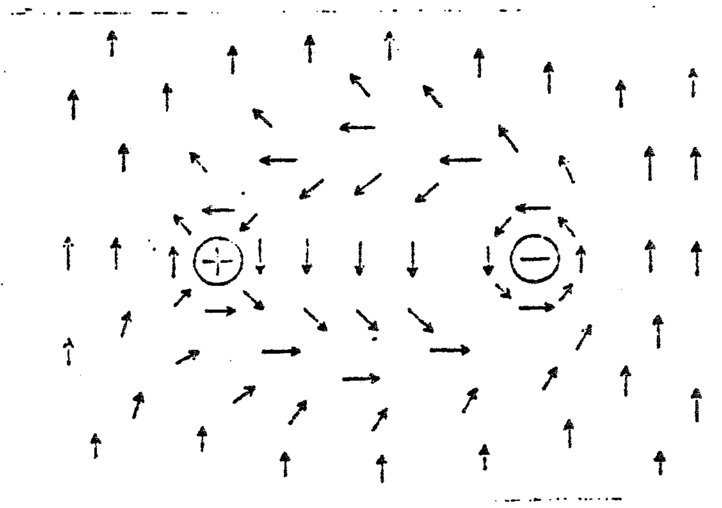


Fig. 3. Spin configuration of a vortex pair.

separation s of the vortices. Close to each vortex the value of v is similar to that of an isolated vortex. It follows that the energy of the pair may be written[27]

$$E_2(s) = 2\pi K_0 \ln(s/a) + \text{const.} \qquad (2.33)$$

Before concluding this discussion, let me make a remark concerning the application of the vortex concept to models where the spins are defined on a lattice of sites, as in Professor Suzuki's talk.[9] When $\vec{S}(\vec{r})$ is defined as a continuous function of $\vec{r}$, vortices may be identified with the places where $\vec{S}(\vec{r}) = 0$, and, of course, no vortices could occur in such a model if $|S(\vec{r})|$ is required to be unity. Vortices can occur in a lattice model, however, even if $|\vec{S}|$ is required to be unity at every lattice site. From the present point of view, we would simply say that a vortex occurs when the interpolated function $\vec{S}(\vec{r})$ vanishes at some point in between the lattice sites. (For an alternative, statistical method of introducing vortices in a lattice spin model, see the work of José et al.[14])

C. Application to superfluidity.

We shall now consider in greater detail applications to superfluidity. Let us define a local superfluid velocity by

$$\vec{v}_s(\vec{r}) \equiv \frac{\hbar}{m} \nabla\phi(\vec{r}) \ . \qquad (2.34)$$

According to the Ginzburg-Landau theory, there will be associated with $\vec{v}_s$ a super-current density or momentum density given by[20,25]

$$\vec{g}_s(\vec{r}) = \frac{\delta H}{\delta v_s(\vec{r})} = \frac{m}{\hbar} J \, |\psi(\vec{r})|^2 \, \vec{\nabla}\phi(\vec{r}) \quad . \tag{2.35}$$

For small values of $\vec{v}_s$, we may set $|\psi(\vec{r})| = \psi_0$. Then

$$\vec{g}_s(\vec{r}) = \rho_s^0 \, \vec{v}_s(\vec{r}) \ , \tag{2.36}$$

$$\rho_s^0 = \left(\frac{m}{\hbar}\right)^2 K_0 \ . \tag{2.37}$$

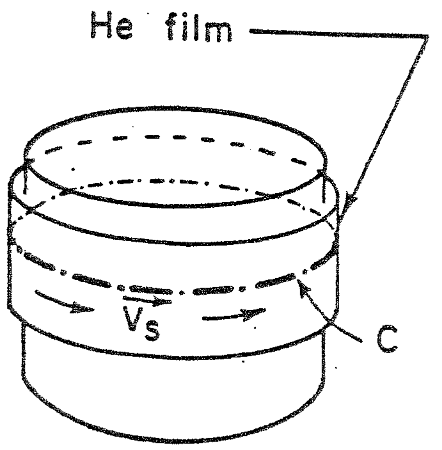
The quantity ρ_s^0 is the bare superfluid density, measured in units of grams per square centimeter. In the present paper we shall use units where $\hbar/m = 1$, so that

$$\rho_s^0 = K_0 \ , \tag{2.38}$$

$$\vec{v}_s = \vec{\nabla}\phi \equiv \vec{v} \ . \tag{2.39}$$

We may now consider the phenomenon of persistent currents. Let us consider a superfluid film wrapped around a cylinder as shown in Fig. 4.

Fig. 4. Superfluid film wrapped around a cylinder.



Suppose that at time t=0 there is a supercurrent flowing in the film. Then if C is a contour which encloses the cylinder, we expect

$$\oint_C \vec{v}_s \cdot d\vec{r} = 2\pi N_C \neq 0 \quad . \tag{2.40}$$

If ψ is different from 0 everywhere in the film, i.e., if there are no vortices present, then we know that

$$dN_C/dt = 0 \quad . \tag{2.41}$$

If free vortices are present, however, then N_C can relax to zero; either by motion of positive vortices from the top to the bottom of the film, or by motion of negative vortices from the bottom to the top. The rate of change of N_C is just equal to the net vortex current flowing across the contour C,[25]

$$\frac{dN_C}{dt} = \oint_C (\hat{z} \times \vec{J}_v) \cdot d\vec{r} \quad , \tag{2.42}$$

where $\hat{z}$ is a unit vector normal to the film. Note that the flow of neutral bound-vortex pairs cannot relax N_C to zero, because the net vortex current $\vec{J}_v$ is zero in that case.

D. Stability against free-vortex formation.

It is clear that the key question for the existence of persistent currents is whether or not there are free vortices present in thermal equilibrium. The question will also be crucial for the issue of whether there is quasi-long range order in the system. A glance at Fig. 2 will suggest that vortices can be very effective in destroying the correlation between spin orientations at different points in the system. It is reasonable to guess that if free vortices are present, then Eq. (2.9) will hold, and the correlation length ξ_+ will be of the order of the mean distance between the free vortices in the system.

Kosterlitz and Thouless have given the following argument concerning the stability of the system against free vortex formation.[4] Let us consider an isolated vortex in a system of radius R. The probability density p_1 for finding such a vortex should be proportional to

$$p_1 = e^{-H_1/T} \quad , \tag{2.43}$$

where H_1 is given by Eq. (2.32). For large values of R, we have

$$p_1 \approx \left(\frac{a_0}{R}\right)^{\pi K_0/T} \quad , \tag{2.44}$$

The total probability of finding an isolated vortex in the system is given by:

$$P = R^2 p_1 \approx R^{2-\pi K_0/T} \tag{2.45}$$

If $(K_0/T) > 2\pi^{-1}$, then $P \to 0$ when $R \to \infty$. If $(K_0/T) < 2\pi^{-1}$, then $P \to 1$ when $R \to \infty$. In order for superfluidity to exist, therefore, we should have

$$\frac{K_0}{T} \geq \frac{2}{\pi} \; , \tag{2.46a}$$

$$\eta \gtrsim \tfrac{1}{4} \; , \tag{2.46b}$$

where the last inequality has been obtained using (2.19). If (2.46) does not hold, entropy will be more important than energy, and free vortices should be present.

Of course, a more careful argument must take into account the interaction between vortices. Note that vortex pairs have finite energy and will be present at all temperatures. However, as we have argued before, vortex pairs in themselves are not enough to destroy superfluidity.

E. Macroscopic description of the low-temperature phase.

Let us now examine in greater detail the effects of an equilibrium density of bound vortices, and of small fluctuations in the magnitude of ψ. In the presence of fluctuation, we must take a spatial average over a region near each point $\vec{r}$, and define a slowly varying order parameter $\Psi(\vec{r})$. We define a slowly varying phase $\Phi(\vec{r})$ as the phase of Ψ, and we define a macroscopic superfluid velocity by

$$\vec{U}_s(\vec{r}) = \vec{\nabla}\Phi(\vec{r}) \quad . \tag{2.47}$$

We define a renormalized stiffness constant K_R by

$$\delta F = \tfrac{1}{2} \int K_R |\vec{U}_s|^2 \, d^2r \tag{2.48}$$

where δF is the increase in free energy due to fluctuations in ϕ. If, in addition to bound vortex pairs and other magnitude fluctuations, there is an isolated vortex at the origin, then the macroscopic phase must obey the equation, for a contour enclosing the origin,

$$\oint \vec{\nabla}\Phi \cdot d\vec{r} = \pm 2\pi \quad . \tag{2.49}$$

By symmetry we expect the phase Φ to change at a uniform rate around any circle centered at the origin, so that

$$|U_s| = 1/r \quad . \tag{2.50}$$

Then, from (2.48), we see that

$$\delta F = \text{const} + \pi K_R \ln (R/a_0) \tag{2.51}$$

It follows that the correct Kosterlitz-Thouless criterion for stability of the superfluid phase is obtained if we replace K_0 in (2.46a) by constant K_R:[4,28,29]

$$K_R \geq \frac{2}{\pi} T \quad . \tag{2.52}$$

We may also argue that the correlation exponent η, defined in Eq. (2.18), is actually determined by the macroscopic or renormalized stiffness constant, and therefore should be given by

$$\eta = \frac{T}{2\pi K_R} \quad , \tag{2.53}$$

instead of Eq. (2.19). Note that (2.46b) still applies as a criterion for stability of the superfluid phase.

In a superfluid, one defines the macroscopic superfluid density ρ_s by

$$\langle \vec{g}_s \rangle = \rho_s \vec{U}_s \tag{2.54}$$

It is possible to show quite generally that for a superfluid in local equilibrium,[25]

$$\rho_s = K_R \quad . \tag{2.55}$$

We shall see below that this relation is indeed true in the present model; that is, we shall check that

$$\langle \vec{g}_s \rangle \equiv \rho_s^0 \langle \vec{v}_s \rangle = K_R \vec{U}_s \quad . \tag{2.56}$$

It should be emphasized that when magnitude fluctuations or vortex pairs are present, the relationship between $\vec{U}_s$ and $\vec{v}_s$ is non-trivial, and in general[30]

$$\vec{U}_s \neq \langle \vec{v}_s \rangle \quad . \tag{2.57}$$

F. Interaction between vortices.

In order to proceed further, we must consider the energy of an array of vortices with charges N_i at positions $\vec{R}_i$. We shall only consider a "neutral" system, where

$$\sum_i N_i = 0 \quad . \tag{2.58}$$

We shall assume that the separation between the vortices are all larger than a core diameter a_0 so that we may neglect the effects of overlap of the vortex cores. We shall also neglect any magnitude fluctuations outside of the vortex cores.

Let us divide $\vec{v}_s$ into two parts:

$$\vec{v}_s(\vec{r}) \equiv \vec{v}_0(\vec{r}) + \vec{v}_1(\vec{r}) \quad , \tag{2.59}$$

where

$$\vec{\nabla} \times \vec{v}_1 = 0 \quad , \tag{2.60}$$

$$\vec{\nabla} \cdot \vec{v}_0 = 0 \quad . \tag{2.61}$$

In view of Eq. (2.26), we must have

$$\vec{\nabla} \times \vec{v}_0 = 2\pi N(\vec{r}) \quad . \tag{2.62}$$

We shall also assume that at the boundaries of the system,

$$v_{0\perp} = 0 \quad . \tag{2.63}$$

where $v_{0\perp}$ is the component of $\vec{v}$ perpendicular to the boundary. In view of (2.60) we may write $\vec{v}_1$ as gradient of a single valued function ϕ_1:

$$\vec{v}_1 = \vec{\nabla}\phi_1 \quad . \tag{2.64}$$

This is possible, even in a multiply connected system, provided that we include in $\vec{v}_0$ any circulation associated with the interior boundaries, or holes in the system. We shall describe $\vec{v}_0$ as the "vortex part" of the superfluid velocity, and $\vec{v}_1$ as the "spin-wave" part.

It is straightforward to show, using (2.61), (2.60) and (2.63) that

$$\int \vec{v}_1 \cdot \vec{v}_0 d^2r = 0 \quad . \tag{2.65}$$

(Substitute (2.64) and integrate by parts). We may now write Eq. (2.13) for the energy H as

$$H = H_v^0 + H_{sw}^0 \quad , \tag{2.66}$$

where H_v^0 and H_{sw}^0 are the vortex and spin wave parts, respectively, given by

$$H_v^0 = \frac{K_0}{2} \int |v_0|^2 d^2r \ + \text{core correction}, \tag{2.67}$$

$$H^0_{sw} = \frac{K_0}{2} \int |v_1|^2 d^2r \quad . \tag{2.68}$$

The core correction in Eq. (2.67) arises because Eq. (2.13) is not valid in the vicinity of the vortex cores where magnitude fluctuation must be taken into account.

We shall see that for a given charge density $N(\vec{r})$, $\vec{v}_0$ is uniquely determined by the conditions of (2.61)-(2.63). The term H^0_{sw} is equal to or greater than 0, and is clearly minimized by the choice $\vec{v}_1 = 0$. The term H^0_v is therefore the minimum energy of the system when the charge density $N(\vec{r})$ is present.

The separation (2.66) implies that the free energy of the system is equal to the sum of the free energies of the vortices and the spin-wave parts separately. The free energy arising from H^0_{sw} is clearly an analytic function of temperature, and will not be of interest to us here.

It is highly desirable to rewrite H^0_v in a more transparent form. For this purpose, we may suppose that $\vec{v}_1 = 0$ and therefore $\vec{v}_s = \vec{v}_0$. Let us define a vector field

$$\begin{aligned} \vec{E}(\vec{r}) &\equiv -2\pi\, K_0\, \hat{z} \times \vec{v}_s(\vec{r}) \\ &= -2\pi\, \hat{z} \times \vec{g}_s(\vec{r}) \end{aligned} \tag{2.69}$$

Note that $\vec{E}(\vec{r})$ is proportional to $\vec{v}_s(\vec{r})$ but rotated 90° in orientation.

In terms of $\vec{E}(\vec{r})$, Eqs. (2.61)-(2.63) may be written[4,27]

$$\vec{\nabla} \times \vec{E} = 0 \quad , \tag{2.70}$$

$$E_{\parallel} = 0 \text{ at boundaries,} \tag{2.71}$$

$$\vec{\nabla}\cdot\vec{E} = \frac{4\pi N(\vec{r})}{\varepsilon_0} \quad , \tag{2.72}$$

where

$$\varepsilon_0 \equiv \frac{1}{\pi K_0} \quad . \tag{2.73}$$

Equations (2.70)-(2.72) are simply Poisson's equations for the electric field due to a static charge distribution $N(\vec{r})$ in a dielectric medium with dielectric constant ε_0, with metallic conductors at the boundaries of the region. As is well known, the electric field is uniquely determined by the charge distribution $N(\vec{r})$ provided that one also knows the total charge of any interior conductors of the region. The energy of the system is given by

$$H_v^0 = \frac{1}{8\pi\varepsilon_0} \int |\vec{E}|^2 d^2r + \text{"core"}$$

$$= \frac{1}{2\varepsilon_0} \sum_{i \neq j} N_i N_j \, G(\vec{R}_i, \vec{R}_j) + \sum_i N_i{}^2 E_c \quad , \qquad (2.74)$$

where $\varepsilon_0{}^{-1} G(\vec{R}_i \vec{R}_j)$ is the electrostatic potential at point $\vec{R}_i$ due to a unit charge at point $\vec{R}_j$. Far away from the boundaries of the system, we may write:

$$G(\vec{R}_i, \vec{R}_j) = -2 \ln\left(\frac{|\vec{R}_i - \vec{R}_j|}{a_0}\right) \quad . \qquad (2.75)$$

We may also define a "force" on the vortex at point R_i by

$$\vec{f}_i \equiv \frac{-\partial H_v}{\partial R_i} = N_i \, \vec{E}(\vec{R}_i) = -2\pi N_i \, \hat{z} \times \vec{g}_s(\vec{R}_i) \quad . \qquad (2.76)$$

Here, $\vec{E}$ is the electric field at point $\vec{R}_i$ due to the other vortices in the system, and to any charges that may exist on the metallic boundaries. We need not include the direct self-field of the vortex at $\vec{R}_i$; that field will be circularly symmetric about $\vec{R}_i$ and will be zero when averaged over the core of the vortex.

Let us suppose that the only other charge in the system is a charge $-N_i$ at the origin, and let us suppose that the boundaries are far away. Then we have

$$\vec{E}(\vec{R}_i) = \frac{-N_i}{\varepsilon_0} \frac{2\vec{R}_i}{|R_i|^2} \qquad (2.77)$$

If in addition to the charge $-N_i$ at the origin we have a thermal distribution of bound vortex pairs, and if R_i is very large but still much smaller than the radius of the system, then we may write

$$<\vec{E}(\vec{R}_i)> \; = \frac{-N_i}{\epsilon_R} \frac{2\vec{R}_i}{|R_i|^2} \tag{2.78}$$

where ϵ_R is the renormalized dielectric constant of the system, taking into account the polarizability of the thermally distributed pairs. Using the definition (2.69) of $\vec{E}$, we see that the supercurrent density at point r arising from a vortex with charge $-N_i$ at the origin is given by

$$<\vec{g}_s(\vec{r})> = \frac{N_i}{\pi\epsilon_R} \; \hat{z} \times \frac{\vec{r}}{r^2} \quad . \tag{2.79}$$

From (2.50) and the definition (2.54) of the macroscopic superfluid density ρ_s it follows immediately that

$$\rho_s = \frac{1}{\pi\epsilon_R} \quad . \tag{2.80}$$

By consideration of the work necessary to move a test vortex a small distance $d\vec{R}_i$ it is apparent that

$$\frac{\partial F}{\partial \vec{R}_i} = -N_i <\vec{E}(\vec{R}_i)> \quad , \tag{2.81a}$$

where F is the free energy of the system. It follows that the free energy of a vortex pair, consisting of a charge N_i at $\vec{R}_i$ and a charge $-N_i$ at the origin, in the presence of a thermal distribution of other (smaller) pairs, is given for large R_i by

$$\delta F = \frac{2|N_i|^2}{\epsilon_R} \; \ln \left(\frac{|R_i|}{a_0}\right) + \text{const.} \tag{2.81b}$$

Comparing with (2.51) we see that

$$\frac{1}{\pi\varepsilon_R} = K_R \quad . \tag{2.82}$$

Comparing (2.80) and (2.82) we verify that $\rho_s = K_R$.

G. The renormalization-group approach.[5,28,29,31]

It is clear that our most important task is to calculate the renormalized dielectric constant

$$\varepsilon_R \equiv \varepsilon_0 + 4\pi\chi \tag{2.83}$$

where χ is the dielectric susceptibility arising from the vortex charges in the system. We shall find that at low temperatures, all vortices are bound in pairs and therefore ε_R is finite. At higher T, free vortices will exist and ε_R will be infinite.

Let us define pairs in the following manner: First, pair up the closest charges of opposite sign, i.e., those with separation in the range $a_0 < r < a_0(1+d\ell)$, with $d\ell$ small. Next, consider the remaining unpaired charges and pair up those in range $a_0(1 + d\ell)<r<a_0(1+d\ell)^2$. In this way we define pairs and we may define a density of pairs $p(r)$ for pairs of separation $\vec{r}$. That is, $p(r)d^2R_+d^2R_-$ is the probability of finding a pair with the positive charge at $\vec{R}_+$ and the negative charge at $\vec{R}_-$ where $r = |\vec{R}_+-\vec{R}_-|$ is the separation of the pair.

If r is fixed and the density of pairs sufficiently small, we may neglect interaction between pairs and write $p \propto \varepsilon^{-E_2(r)/T}$ where E_2 is the energy of an isolated pair and is given by Eq. (2.33). We therefore find

$$p(r) \approx p_0(r) = \left(\frac{1}{a_0}\right)^4 y_0{}^2\left(\frac{a_0}{r}\right)^{2\pi K_0/T} \quad , \tag{2.84}$$

where y_0 is a dimensionless "fugacity" of the vortices. We may write

$$y_0 = n_0 e^{-E_c/T} \quad , \tag{2.85}$$

where n_0 is the number of independent places to put a vortex in a cell the size of $a_0{}^2$, and E_c is the vortex core energy.

We are actually interested in the behavior of p in the limit $r\to\infty$ for fixed y_0. We wish to take into account screening of interaction between the members of a pair separated by r, arising from the thermal distribution of pairs with $r' \ll r$. Let us define the dielectric constant $\varepsilon(r)$ as the dielectric constant including just the polarizability of pairs with separation less than r. We calculate the functions $\varepsilon(r)$ and $p(r)$ by iterative increments of r, and we arrive at the following equations:

$$\varepsilon(r+dr) = \varepsilon(r) + 4\pi\ \frac{r^2}{2T}\, 2\pi r\ p(r)\ dr \quad , \tag{2.85}$$

$$p(r+dr) = p(r)\exp\left[\frac{-2}{rT\varepsilon(r)}\,dr\right] \quad . \tag{2.86}$$

In (2.85) the factor $\frac{r^2}{2T}$ is just the polarizability of a pair with separation r. The factor $2\pi r p(r)dr$ is just the number of pairs per unit area with separation in the range between r and r+dr. The argument of the exponential in (2.86) is just -1/T times the work done in increasing the separation of the pair by the amount dr. The starting values of ε and p are given by

$$\varepsilon(r=a_0) = \varepsilon_0 \quad , \tag{2.87}$$

$$p(r=a_0) = y_0{}^2/a_0{}^4 \quad . \tag{2.88}$$

We want to calculate

$$\varepsilon_R = \varepsilon(r=\infty) \quad . \tag{2.89}$$

It is helpful to introduce dimensionless variables:

$$\ell \equiv \ln\,(r/a_0) \quad , \tag{2.90}$$

$$[y(\ell)]^2 \equiv r^4\ p(r)\big|_{r=a_0e^{\ell}} \quad , \tag{2.91}$$

$$\tilde{K}(\ell) \equiv \frac{K(\ell)}{T} \quad . \tag{2.92}$$

polarization $q\vec{r}$

distance between particles

$* \quad V = -\vec{P}\cdot\vec{E} = -pE\cos\theta = -q\,r\cos\theta\,E = -r\cos\theta\,E$

$P = r\,\overline{\cos\theta}\ ; \quad \overline{\cos\theta} = \frac{\int e^{-V/kT}\cos\theta\,d\theta}{\int e^{-V/kT}\,d\theta} \qquad \frac{\int e^{\cos\theta\,(rE/T)}\cos\theta\,d\theta}{\int e^{\cos\theta\,(rE/T)}\,d\theta} = \frac{d}{da}\log\left[\int e^{a\cos\theta}\,d\theta\right]$

polarization

where

$$\tilde{K}(\ell) = \frac{1}{\pi\varepsilon(r)}\Big|_{r=a_0e^{\ell}} \tag{2.93}$$

Equations (2.85) and (2.86) may now be written

$$\frac{d\tilde{K}^{-1}}{d\ell} = 4\pi^3y^2 + O(y^4) \tag{2.94}$$

$$\frac{dy}{d\ell} = [2-\pi\tilde{K}]y + O(y^3) \tag{2.95}$$

These are the famous Kosterlitz recursion relations.[5] We have written explicitly the correction terms in (2.94) and (2.95) to remind us that the derivation of these equations is only valid when $y(\ell)$ is small. The correction terms arise when several pairs are present such that the separation between the pairs is of the same order of magnitude as the separation of the members of the pair, and therefore nonlinear interactions must be considered.

We may note from Eq. (2.95) that y decreases with increasing ℓ when $\tilde{K} > 2\pi$, It is convenient to introduce a variable

$$x \equiv \left(\frac{2}{\pi}\tilde{K}^{-1}-1\right) \tag{2.96}$$

Near the transition (where $x = 0$), the Kosterlitz equations become

$$\frac{dx}{d\ell} = 8\pi^2y^2 \tag{2.97}$$

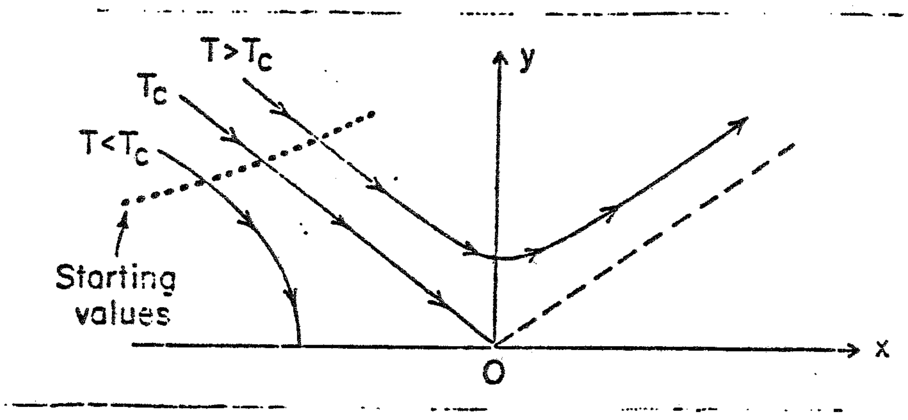
$$\frac{dy}{d\ell} = 2xy \tag{2.98}$$

The flow diagram for these equations is indicated in Fig. 5.

$\simeq \frac{d}{da} \log \left[\int 1 + \cos\theta\, a + \frac{1}{2}\cos^2\theta\, a^2 + \cdots\right]$ [illegible]

$\simeq \frac{d}{da}\left[\log 2\pi + \log\left(1 + \frac{1}{4}a^2\right)\right] = \frac{1}{2}a \Rightarrow P = \frac{r^2}{2T}E$

Fig. 5. Flow diagram for Kosterlitz recursion relations.



Although an analytic solution of Eqs. (2.97) and (2.98) can be given,[9,10] it will suffice for our purposes to describe some general features of the solution. Equations (2.97) and (2.98) have an integral:

$$x^2 - 4\pi^2 y^2 = x_0{}^2 - 4\pi^2 y_0{}^2, \qquad (2.99)$$

where x_0 and y_0 are the starting values of x and y. At $T=T_c$, the right-hand side of (2.99) vanishes, and the trajectory for x and y is a straight line coming into the origin. Along this line, we have

$$y = \frac{-x}{2\pi} \sim \frac{1}{4\pi\ell} = \frac{1}{4\pi \ln(r/a_0)} \quad . \qquad (2.100)$$

It follows that for $T=T_c$,

$$\tilde{K}_R = K_R/T = 2/\pi \quad , \qquad (2.101)$$

$$\varepsilon_R = 1/2T_c \quad , \qquad (2.102)$$

$$p(r) = y^2/r^4 = 1/r^4 \ln^2 r \quad . \qquad (2.103)$$

From (2.101) we see that the inequalities (2.52) and (2.46b)become equalities at T_c.

Since the starting values x_0 and y_0 are analytic functions of temperature T, the right-hand side of (2.99) should be proportional to T_c-T, sufficiently close to the transition. For $T < T_c$, Eq. (2.99) is positive and $y \to 0$ for large values of ℓ. It follows that

$$\tilde{K}_R = \frac{2}{\pi} + b|T_c-T|^{\frac{1}{2}} \quad , \tag{2.104}$$

where b is a constant that depends on the details of the system.

For T slightly greater than T_c, $y(\ell)$ first decreases with ℓ and then begins to increase. One finds that $y(\ell)$ will reach a value of order magnitude unity when ℓ has the value

$$\ell \equiv \ell_T = \frac{1}{b(T-T_c)}{}^{\frac{1}{2}} + \text{const.} \tag{2.105}$$

At this point, the Kosterlitz recursion relations no longer make sense. For a length-scale $r \geq a_0 e^{\ell T}$ it does not make sense to consider pairs. We believe that the remianing vortices are essentially free, i.e., they behave like charges in a conventional plasma. The density of these charges will be given by

$$n_{\text{free}} = \frac{1}{(a_0 e^{\ell T})^2} \approx \exp\left(\frac{-2}{b|T-T_c|^{\frac{1}{2}}}\right) \quad . \tag{2.106}$$

We may define a plasma screening length k_s^{-1}, which should be given, at least approximately, by the Debye formula:

$$k_s^2 = 4\pi n_{\text{free}}/T\varepsilon_b \quad , \tag{2.107}$$

where ε_b is the dielectric constant due to the bound pairs. As an approximation, we may equate ε_b to the renormalized dielectric constant at T_c:

$$\varepsilon_b \approx \varepsilon_R\ (T=T_c) = \tfrac{1}{2}T_c^{-1} \ . \tag{2.108}$$

Using these approximations, we find

$$k_s^2 \approx 8\pi n_{\text{free}} \quad . \tag{2.109}$$

At temperature $T > T_c$ we expect that the order parameter correlation function should decay exponentially at large distances according to Eq. (2.9). More precisely, we expect that the correlation function will have Ornstein-Zernike form, which in two dimensions is[21]

$$<\psi^*(r)\psi(o)> \sim \frac{e^{-r/\xi^+}}{r^{\frac{1}{2}}} \quad . \tag{2.110}$$

As was mentioned earlier, we may estimate the correlation length as the mean distance between free vortices, so that

$$\xi_+ = (n_{free})^{\frac{1}{2}} \approx (8\pi)^{\frac{1}{2}} k_s^{-1} \quad . \tag{2.111}$$

Other arguments, which will not be given here, suggest that there is a precise relation[10]

$$\xi_+ = 2k_s^{-1} \quad . \tag{2.112}$$

Note that the distinction between bound pairs and free vortices is not a precise one, and we do not know how to define n_{free} in a precise way. Nevertheless, the temperature-dependence of n_{free} is well defined, and we may write

$$\xi_+ \propto \exp\left(\frac{1}{b|T-T_c|^{\frac{1}{2}}}\right) \quad . \tag{2.113}$$

The renormalization group approach may also be used to study the singular part of the free energy near T_c. A scaling argument suggests that the singular part of the free energy should vary as ξ^{-2}. In view of (2.113), this means that the singular part of the free energy and all of its derivatives vanish as T approaches T_c. Therefore, *the specific heat and all of its derivatives* should be *continuous* at the Kosterlitz-Thouless transition; one cannot locate the transition temperature by any structure in the specific heat or other thermodynamic properties. The phase transition *can* be seen if one studies the long wavelength elastic constant K_R or superfluid density ρ_s, which vanish discontinuously as one passes through T_c. Also, the large distance behavior of the order parameter correlation function changes from quasi-long range behavior to short range behavior precisely at $T=T_c$.

The relation (2.101) for K_R/T_c may be tested experimentally by measurement of the areal superfluid density ρ_s at the transition temperature of a thin helium film. (The importance of this relation as a test of the theory has been emphasized by Nelson and Kosterlitz,[28] who showed that (2.101) is exact in the renormalization group theory.) Measurements have been made by a variety of techniques on films containing ^{3}He impurities, and films of pure ^{4}He, over a considerable range of transition temperatures. These measurements are consistent with (2.101) within the accuracies of the experiments, which are typically of order ± 15%. (See Refs. 32-34.)

The Kosterlitz renormalization group method does not really answer the question of whether any given system, such as, for example, the nearest neighbor X-Y model, or a helium film of particular thickness, actually has a transition of the Kosterlitz-Thouless type. In particular, we cannot rule out the possibility that the phase transition might occur by some totally different machanism or by a first-order transition before the Kosterlitz-Thouless temperature is reached.[35] In general, the starting value y_0 is of order unity, and the Kosterlitz recursion relations are not very accurate for small values of ℓ. If the Kosterlitz equations are even qualitatively correct in this region, however, the system will flow into the region where $y(\ell)$ is very small, and the predictions of the Kosterlitz theory should then apply precisely, in the vicinity of the transition temperature. (Again, provided that some other type of transition does not occur first.) Regardless of the mechanism of the transition, however, the inequalities (2.52) and (2.46b) should apply as a criterion for stability everywhere in the superfluid phase.[36]

H. Comment on the two-dimensional Heisenberg model.

It is interesting to compare the behavior of the planar-spin model discussed above with that of the two-dimensional Heisenberg model. The Heisenberg model is characterized by a three component order parameter,

$$\vec{S} = (S_x, S_y, S_z) \quad , \tag{2.114}$$

whose magnitude may be taken to be unity. We may write the Hamiltonian of the Heisenberg model in a continuum limit as

$$H = \tfrac{1}{2} \int d^2r \, K_0 |\vec{\nabla} S|^2 \quad . \tag{2.115}$$

Following the analysis of Polyakov,[2] we believe that the elastic constant K is renormalized to 0 at long wavelengths, for any temperature greater than 0. This will occur even without fluctuation of the magnitude of $\vec{S}$. The conclusion is that there is no quasi-long range order in the two-dimensional Heisenberg model, and no phase transition at any temperature greater than 0.

The physical reason for this behavior is that two angles are necessary to specify the orientation of S in the Heisenberg model. In polar coordinates, we specify the polar angle θ and the azimuthal angle ϕ. Fluctuations of these two angles interact strongly, and this interaction is responsible for the renormalization calculated in Polyakov's theory. If the polar angle θ is very close to 0 or π, then the energy associated with gradients in ϕ is very small. If the polar angle reaches 0 or π at any point, the value of ϕ will generally be discontinuous at that point, and the value of ϕ changes by $\pm 2\pi$ if one follows a contour enclosing the point. Thus, even without magnitude fluctuations, it is generally impossible to define ϕ to be continuous and single valued. It can be shown that these configurations, which play the role of a vortex in the field ϕ, do not have a divergent energy in the Heisenberg model.

I believe that either of the two effects described above, the strong interactions of fluctuations in the angles, or the absence of a divergent energy for vortex-like configurations, is sufficient to destroy the quasi-long range order, at $T \neq 0$.

3. DYNAMICS OF SUPERFLUID FILMS

A. Equations of motion for $\vec{v}_s$.

I shall now discuss the dynamics of a very thin superfluid film close to its transition temperature. Using Eqs. (2.24)-(2.27), we may write for a general contour C,

$$\int_C \frac{d\vec{v}_s}{dt} \cdot d\vec{r} = 2\pi \frac{d}{dt} N_C = -2\pi \int_C (\hat{z} \times \vec{J}_v) \cdot d\vec{r} \quad . \tag{3.1}$$

Thus we may write

$$\frac{\partial \vec{v}_s}{\partial t} + 2\pi \hat{z} \times \vec{J}_v = -\vec{\nabla} \Xi \tag{3.2}$$

where Ξ is an unknown single-valued function of position. Far away from any vortex core $\vec{J}_v = 0$, and we expect that the Josephson relation[25] should hold,

$$\frac{d\phi}{dt} = \frac{-\hbar}{m}\mu \quad , \tag{3.3}$$

$$\frac{d\vec{v}_s}{dt} = -\nabla\mu \quad , \tag{3.4}$$

where μ is the chemical potential. It follows that $\Xi = \mu$ far away from vortex cores, and we shall make the approximation that this relationship holds everywhere outside of the vortex cores. We shall also assume that the temperature is a constant in the film. (This last assumption is correct, in particular, if thermal contact to the substrate is sufficiently good.) Under these circumstances, we may write:

$$d\mu = \frac{d\rho}{\chi_\rho} \quad , \tag{3.5}$$

where ρ is the helium mass per unit area and the coefficient χ_ρ is determined by the Van-der Waals force between helium and the substrate.[37]

From the above consideration, we arrive at the equation of motion:

$$\frac{d\vec{v}_s}{dt} = \frac{-\vec{\nabla}\rho}{\chi_\rho} - 2\pi\,\hat{z} \times \vec{J}_v \quad . \tag{3.6}$$

Also, if we assume that there is no evaporation of helium into the vapor, we have conservation of mass in the film, and we may write:

$$\frac{\partial\rho}{\partial t} = -\rho_s^0\, \nabla\cdot\vec{v}_s \quad . \tag{3.7}$$

Finally, from Eq. (2.26), we have

$$\nabla \times \vec{v}_s = 2\pi\, N(\vec{r}) \quad . \tag{3.8}$$

B. Analogy with Maxwell's equations.[10]

Let us define the quantity

$$\vec{B}(r) = 2\pi\,\hat{z}\,\delta\rho(\vec{r}) \quad , \tag{3.9}$$

where $\delta\rho$ is the deviation of the areal density of helium from its average density in the film. We define the vector field $\vec{E}$ as in Eq. (2.69). Equations (3.6)-(3.8) may now be written

$$\varepsilon_0 \frac{\partial\vec{E}}{\partial t} = \mu_0^{-1}\,\vec{\nabla}\times\vec{B} - 4\pi\vec{J}_v \tag{3.10}$$

$$\frac{\partial\vec{B}}{\partial t} = -\vec{\nabla}\times\vec{E} \tag{3.11}$$

$$\varepsilon_0\vec{\nabla}\cdot\vec{E} = 4\pi N \tag{3.12}$$

where ε_0 is defined by Eq. (2.73) and

$$\mu_0 = \pi\chi_\rho \quad . \tag{3.13}$$

But these equations, (3.10)-(3.12), are identical to Maxwell's equations for a two-dimensional system with a bare dielectric constant ε_0 and a magnetic permeability μ_0! [The fourth Maxwell equation, $\vec{\nabla}\cdot\vec{B} = 0$, follows trivially from Eq. (3.9), since $\vec{B}$ depends only on the coordinates x and y.]

C. Motion of vortices

If we set $J_v = 0$, Eqs, (3.10)-(3.12) have a wave solution (third sound[37]) with a velocity c_0 given by

$$c_0^2 = \frac{1}{\varepsilon_0\mu_0} = \frac{\mu_s^0}{\chi_\rho^0} \tag{3.14}$$

More generally, one must take into account the flow of the vortices. We shall assume the following equation of motion:[10,38]

$$\frac{d\vec{R}_i}{dt} = \frac{D}{T}\vec{f}_i + (1-C)\vec{v}_s + \text{noise} \tag{3.15}$$

where $\vec{f}_i$ is the force on the i^{th} vortex, defined by Eq. (2.76):

$$\vec{f}_i = N_i\vec{E}(\vec{R}_i) = -2\pi N_i\rho_s^0\,\hat{z}\times\vec{v}_s \quad . \tag{3.16}$$

In (3.15) the coefficient $\frac{D}{T}$ is the <u>mobility</u> of the vortex which we have related to the diffusion constant D by means of the Einstein relation. The noise term is a Brownian motion consistent with this diffusion constant. The constant C is a number in the range $0 < C < 1$. We have assumed here that the substrate is at rest, and therefore that the normal fluid velocity $\vec{v}_n$ is zero.

At T=0, on an ideal smooth substrate, when no normal fluid is present, one finds that

$$C = D = 0 \quad . \tag{3.17}$$

In this case, there is no noise or dissipation and the vortex is simply carried along with the local superfluid velocity. On the other hand, if there is strong friction opposing the motion of the vortices, either because of interaction with the substrate or because of strong scattering of normal fluid,

$$C \approx 1 \quad . \tag{3.18}$$

In this case, the vortex moves in the direction of the force $\vec{f}$, (i.e., perpendicular to the superfluid velocity $\vec{v}_s$). The non-dissipative motion parallel to the superfluid velocity, which occurs when $C \neq 0$, is of little consequence for problems that we are considering, and in fact the term proportional to C will not enter at the level of the approximations that we will be making.

The value of the diffusion constant D reaches a maximum for moderate values of the friction, and one finds that [10]

$$\text{Maximum } D \approx \hbar/m = 10^{-4}\text{cm}^2/\text{sec}. \tag{3.19}$$

Arguments can be given that there is no divergent renormalization of D in the neighborhood of T_c.[39]

D. <u>Linear response at finite ω.</u>[10]

For small deviations from equilibrium, at a finite frequency ω, the system can be described by linear response theory. Let us define a frequency-dependent dielectric constant $\varepsilon(\omega)$ by

$$\frac{4\pi i}{\omega} \langle \vec{J}_v \rangle = (\varepsilon-\varepsilon_0) \langle \vec{E} \rangle \tag{3.20}$$

(It is a very good approximation to neglect the wave vector-dependence of ε.) Our task will be to estimate the form of $\varepsilon(\omega)$.

Once $\varepsilon(\omega)$ is known, we may write the wave equation for modes with transverse $\vec{E}$ (i.e., longitudinal $\vec{v}_s$):

$$k^2 = \omega^2 \mu_0 \, \varepsilon(\omega) \quad . \tag{3.21}$$

In a frequency range where $\varepsilon(\omega)$ is real, or nearly real, we will find a real value of k corresponding to a propagating mode. For a frequency where $\varepsilon(\omega)$ is close to the imaginary axis, we will find an overdamped or diffusive mode. One may also look for "plasma modes" with longitudinal $\vec{E}$ (transverse $\vec{v}_s$) by solving the equation

$$\varepsilon(\omega) = 0 \quad . \tag{3.22}$$

Let us write:

$$\varepsilon(\omega) = \varepsilon_b(\omega) + \frac{4\pi i}{\omega} \sigma_v \quad , \tag{3.23}$$

where $\varepsilon_b(\omega)$ is the contribution of the bound charges, and σ_v is the conductivity of the free charges (vortices):

$$\sigma_v \approx n_{free} \, D/T \quad . \tag{3.24}$$

For $T > T_c$ we may approximate

$$\varepsilon_b \approx \varepsilon_R(T_c) = \frac{1}{2T_c} \quad . \tag{3.25}$$

One then finds for $\omega \gg Dn_{free}$, that

$$\varepsilon(\omega) = \varepsilon_R(T_c) \quad . \tag{3.26}$$

[A more accurate estimate of $\varepsilon(\omega)$ in this regime may be obtained from Eq. (3.37) below.] We see that 3rd sound propagates in this frequency range, with approximately the same velocity as at $T = T_c$.

For $\omega << Dn_{free}$, the second term on the right-hand side of (3.23) is dominant, and we may write

$$\varepsilon(\omega) \approx 4\pi i\, \sigma_V/\omega \quad . \tag{3.27}$$

In this region, the solution of Eq. (3.21) is a diffusive mode with

$$\omega = -i\left(\frac{\lambda}{\chi_\rho}\right)k^2 \quad . \tag{3.28}$$

The coefficient λ is the mass transport coefficient for the helium in the film, and it has the temperature dependence

$$\lambda \propto (n_{free}\; D/T)^{-1} \propto \xi_+{}^2 \quad . \tag{3.29}$$

It is interesting to note that the temperature dependence in (3.29) is a stronger divergence than is predicted by the dynamic scaling theory, $\lambda \propto \xi^{\frac{1}{2}(4-d)}$, which would have λ proportional to ξ_+, near the superfluid transition in two dimensions.[41,42]

From Eq. (3.22) we find a relaxational mode for transverse $\vec{v}_s$, at long wavelengths, at the frequency

$$i\omega = \frac{4\pi\sigma_V}{\varepsilon_b} \equiv \gamma \propto n_{free} \quad . \tag{3.30}$$

This corresponds to a relaxation equation for a divergence-free $\vec{v}_s$:

$$\frac{d\vec{v}_s}{dt} = -\gamma\vec{v}_s \quad . \tag{3.31}$$

E. Third-sound propagation.[10]

For $T \leq T_c$, the second term on the right-hand side of (3.23) is absent, since

$$n_{free} = 0 \quad . \tag{3.32}$$

We now write

$$\varepsilon(\omega) = \varepsilon_b(\omega) = \varepsilon_0 + \int_{a_0}^{\infty} dr \, \frac{d\varepsilon(\omega)}{dr} \quad , \tag{3.33}$$

where $d\varepsilon(\omega)/dr$ is the contribution from bound pairs of separation r. We shall make the approximation

$$\frac{d\varepsilon(\omega)}{dr} \cong \frac{d\varepsilon(r)}{dr} \, \frac{1}{1-i\omega\tau_r} \quad , \tag{3.34}$$

where $d\varepsilon(r)/dr$ is the contribution to the static dielectric function $\varepsilon(r)$ defined in Sec. 2, and τ_r is a characteristic relaxation time for pairs of separation r. One would guess that τ_r is of the order of magnitude of the time necessary for a vortex to diffuse a distance r. Actually, Ambegaokar and Teitel[40] have studied the Fokker-Planck Equation for the separation of a bound pair, and found that the best fit to a single relaxation time approximation is given by

$$\tau_r \approx \frac{r^2}{14D} \quad . \tag{3.35}$$

The form of $d\varepsilon(r)/dr$ may be obtained from the solution of the Kosterlitz equations given in Sec. 2. Close to T_c for large r, $d\varepsilon(r)/dr$ varies approximately as 1/r. It is then a very good approximation in the integral (3.33) and (3.34) to set

$$\mathrm{Re}\left(\frac{1}{1-i\omega\tau_r}\right) \simeq \begin{Bmatrix} 1, \text{ for } \omega\tau_r<1 \\ 0, \text{ for } \omega\tau_r>1 \end{Bmatrix} \quad . \tag{3.36}$$

Hence,

$$\mathrm{Re}\ \varepsilon_b(\omega) = \varepsilon(r)\Big|_{r\,=\,(14D/\omega)^{1/2}} \tag{3.37a}$$

For the imaginary part of ε_b, the integral (3.33) is dominated by values of r close to $(14D/\omega)^{1/2}$. One finds

$$\mathrm{Im}\ \varepsilon_b(\omega) = \frac{\pi}{4}\left[r\cdot\frac{d\varepsilon(r)}{dr}\right]\Big|_{r\,=\,(14/D\omega)^{1/2}} \tag{3.37b}$$

Using the results of Sec. 2, we may now compute the real and imaginary parts of $\varepsilon_b(\omega)$ in various regions of interest. For $T = T_c$ we find

$$\frac{\mathrm{Im}\ \varepsilon(\omega)}{\mathrm{Re}\ \varepsilon(\omega)} \simeq \frac{\pi}{2\ \ln^2(14D/\omega)} \quad . \tag{3.38}$$

Using (3.21), we see that the ratio between the imaginary and real of the third-sound wave-vector k is proportional to (3.38). This ratio approaches 0, when $\omega \to 0$, so that 3rd sound propagates reasonably well at T_c.

For $T < T_c$, in the limit $\omega \to 0$, we find

$$\frac{2\ \mathrm{Im}\ k}{\mathrm{Re}\ k} = \frac{\mathrm{Im}\ \varepsilon(\omega)}{\mathrm{Re}\ \varepsilon(\omega)} \propto \omega^{\pi\tilde{K}_R - 2} \quad , \tag{3.39}$$

where, according to Eq. (2.104):

$$\pi\tilde{K}_R - 2 \propto (T_c - T)^{1/2} \quad . \tag{3.40}$$

Again, the ratio (3.39) goes to 0 in the limit $\omega \to 0$, so that 3rd sound propagates at long wavelengths; however, for T close to T_c the damping predicted by (3.39) and (3.40) is anomalously large compared to the conventional "hydrodynamic" result for the ratio of the attenuation rate to the wave-vector of a superfluid wave:[43,44]

$$\frac{2\ \mathrm{Im}\ k}{\mathrm{Re}\ k} \propto \omega \tag{3.41}$$

Dissipation arising from the oscillatory motion of vortices, (either thermally excited bound pairs or nonequilibrium trapped vorticity), may account for some of the anomalous dampings that have been observed experimentally in thin helium films close to their transition temperatures.[45]

It should be mentioned that in real helium films, the damping of 3rd sound may be complicated by evaporation of atoms from the film and by deviations from the assumed constant temperature. These effects have been studied by Bergman in the absence of vortex motion.[44] It is relatively straightforward to combine Bergman's analysis with the present considerations of dissipation due to vortices.

F. Oscillating substrate experiment

Bishop and Reppy have measured the moment of inertia and dissipation of a helium film on an oscillating substrate.[32] (See also Webster,et al.[33]) This experiment may be analyzed by assuming that Eqs. (3.15) holds in the instantaneous rest-frame of the substrate, and then making a Galilean transformation to the laboratory frame. We find that the momentum-density of the helium is given by

$$\vec{g} = [\rho-\rho_s(\omega)]\vec{v}_n \tag{3.42}$$

where $\vec{v}_n$ is the normal fluid velocity, identical to the velocity of the substrate, and $\rho_s(\omega)$ is a frequency-dependent superfluid velocity, related to the frequency-dependent dielectric constant discussed above, by

$$\rho_s(\omega) \equiv \frac{1}{\pi\varepsilon(\omega)} \tag{3.43}$$

(We have assumed here that v_n is small so that linear response theory may be used.) The quantity $\rho_s(\omega)/\rho$ is the fraction of the helium mass which does not participate in the substrate motion.

In the limit $\omega \to 0$, $\rho_s(\omega)$ is just the static superfluid density ρ_s, which jumps discontinuously to 0 as T passes through T_c, according to the results of Sec. 2. For measurements at finite frequencies, the effective superfluid density $\rho_s(\omega)$ will drop towards 0 at a temperature slightly above T_c. Dissipation in the Bishop-Reppy experiment is proportional to ω times the imaginary part of $1/\varepsilon(\omega)$. For a given $\omega > 0$, the dissipation passes through a maximum as a function of temperature, at a temperature slightly above T_c.

6. Nonlinear relaxation of v_s.

According to the linear response formulae, the dissipation vanishes in the limit $\omega\to 0$, for $T < T_c$, because no free vortices are present. However, if $\omega\to 0$ with a fixed finite value of $\vec{v}_s$, we will actually find a finite value of n_{free} due to "field ionization" of vortex pairs.[25] In the presence of a uniform superfluid momentum density $\vec{g}_s$, the free energy of a pair of vortices is given by

$$F(\vec{r}) = 2\pi K_R \ln(\frac{r}{a}) - \vec{E}\cdot\vec{r} \quad , \tag{3.44}$$

where the electric field $\vec{E}$ is related to $\vec{g}_s$ by Eq. (2.69). The shape of this curve is indicated in Fig. 6.

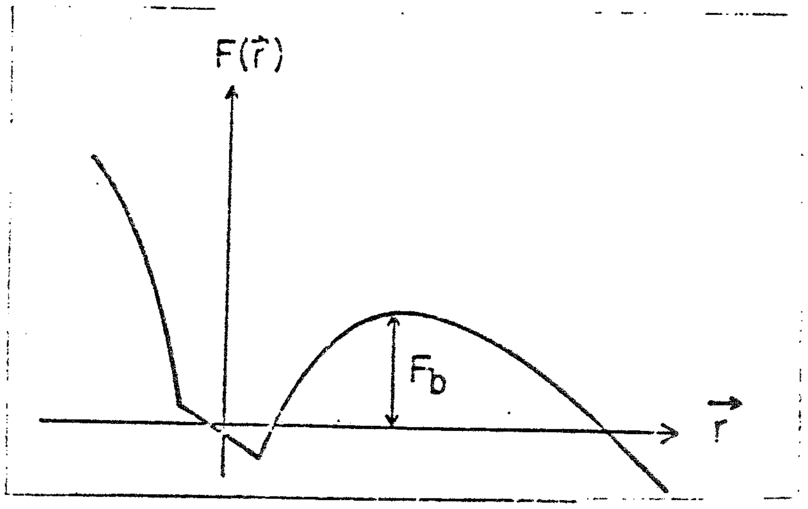


Fig. 6. Free energy of a vortex pair in the presence of a uniform background superfluid velocity, shown as a function of separation $\vec{r}$, for $\vec{r}$ perpendicular to the flow.

Note that the free energy decreases linearly with r for separations in the direction of the electric field. It will be favorable for the pair to separate to infinity, if it surmounts a barrier whose height is given by

$$F_b = 2\pi K_R |\ln E| \ . \tag{3.45}$$

An important factor in the escape rate will be the activation factor [10-13,46-49]

$$e^{-F_b/T} \propto v_s^{2\pi\tilde{K}_R} \quad . \tag{3.46}$$

Actually, the problem must be treated with some care close to T_c, because the pre-exponential factors may also lead to a dependence on v_s comparable to (3.46). In fact, one finds a generation rate for free vortices by ionization of pairs which is given by [10,11,50]

$$\frac{dn_{free}}{dt} = R \propto (T_c - T) v_s^{2\pi\tilde{K}_R} \tag{3.47}$$

In a steady state this generation rate will be balanced by pair recombination of the form

$$-\frac{dn_{free}}{dt} \propto (n_{free})^2 \quad . \tag{3.48}$$

We are thus led to a free vortex density[10-13,49]

$$n_{free} \propto R^{\frac{1}{2}} \quad . \tag{3.49}$$

(A similar final result is obtained if one takes into account the creation and annihilation of vortices at the edges of the film.) Generalizing Eq. (3.31), we find a relaxation rate for the superfluid velocity

$$\frac{1}{v_s}\ \frac{dv_s}{dt} \propto n_{free} \propto (T_c - T)^{\frac{1}{2}}\ v_s^{\pi\tilde{K}_R} \quad , \tag{3.50}$$

where according to Eq. (2.104)

$$\pi\tilde{K}_R = 2 + \pi b|T_c - T|^{\frac{1}{2}} \quad . \tag{3.51}$$

Note that the decay rate (3.50) is nonzero, for any finite value of v_s. However, the decay rate goes to 0, for $\vec{v}_s \to 0$, at least as fast as v_s^2. [In three dimensions, for $T < T_c$, the decay rate is also finite, for finite values of v_s. However, the decay goes to zero more rapidly in the three-dimensional case, roughly proportional to e^{-1/v_s}.[48]]

H. Applications to *superconducting* films.

Our analysis of the static and dynamic properties of the superfluid transition in helium films is applicable, with some modifications, to thin "dirty" superconducting films, in particular to films whose electrical resistance is of the order of several thousand ohms per square or greater.[51-53] In principle, the free energy of a vortex in a superconducting film is finite, rather than logarithmically divergent, because of screening by the three-dimensional magnetic field.[54] There should be no true phase transition in the superconducting film, and the resistivity is finite at all temperatures.[6] In practice, however, the coupling to the three-dimensional magnetic field is quite weak in the systems of greatest interest, and the magnetic screening length is of the order of 1 cm., typically larger than the size of the sample. A superfluid-type analysis may then be applicable over a wide range of temperature. [In the superconducting case, however, it is quite important to take into account the temperature dependence of the Ginzburg-Landau parameter α in Eq. (2.1).] Experimentally, it is necessary to carefully screen out external magnetic fields if one wishes to see the Kosterlitz-Thouless effects arising from vortices of thermal origin.[53]

The mass transport coefficient λ which appears in Eq. (3.29) should be interpreted in the superconducting case as the electrical conductivity of the film.

I. Thick helium films.

The theory of the superfluid transition in two-dimensions, discussed in these lectures, is applicable in principle to helium films of arbitrary thickness, provided we limit our attention to a region sufficiently close to the transition temperature.

Note that the superfluid density ρ_s which enters the Kosterlitz-Thouless-Nelson criterion, Eqs. (2.52) and (2.55) and which appears repeatedly in the present paper, is the integrated superfluid density, with dimensions of mass per unit area. The volume superfluid density $\rho_s^{(3)}$, is given by

$$\rho_s^{(3)} = \rho_s/h \tag{3.52}$$

where h is the thickness of the film. For thick films the transition temperature approaches the bulk transition temperature T_λ; the Kosterlitz-Thouless-

Nelson criterion predicts a jump in $\rho_s^{(3)}$ which vanishes in the limit $h\to\infty$, consistent with the three-dimensional theory.

The width of the temperature region where two-dimensional fluctuations are dominant, and where behaviors such as those in Eqs. (2.104), (2.113), (3.29), (3.30) and (3.50) may be observed, is comparable in magnitude to the depression of T_c due to the finite thickness of the film, $\Delta T \propto h^{-3/2}$. In this temperature interval, the bulk correlation length is comparable to or larger than the thickness of the film.

For a further discussion of this point, see Appendix C of Ref. 10.

4. EFFECT OF A SYMMETRY-BREAKING PERTURBATION

It is very interesting to investigate the effects of adding to the X-Y model Hamiltonian a term of the form

$$H_p = -h_p \int \cos p\phi(\vec{r})\ d^2r \tag{4.1}$$

where p is an integer. Although such a term cannot exist in a superfluid, terms of this form will exist when the order parameter $\vec{S}$ refers to the orientation of a spin or the orientation of a molecule absorbed on a crystalline substrate. Some important cases are:

$p = 1$, representing a magnetic field coupled linearly to $\vec{S}$;

$p = 6$, representing the effects of coupling to a hexagonal substrate;

$p = 2$, representing a uniaxial substrate; and

$p = 4$, representing a square substrate.

If we take the limit $h_p \to \infty$ in Eq. (4.1), the angle ϕ is restricted to values $2\pi n/p$ where n is an integer. This is the p-state "clock model" or the "discrete planar-rotator model," which was used in the Monte Carlo calculations, described by Prof. Suzuki.[9]

The renormalization group method of Sec. 2 can be generalized to this model when h_p is small.[14] We must now consider recursion relations for the renormalized field $h_p(\ell)$ in addition to the variables $y(\ell)$ and $\tilde{K}(\ell)$ considered in Sec. 2. The recursion relation for h_p is

$$\frac{dh_p}{d\ell} = [2 - \frac{p^2}{4\pi\tilde{K}}]\ h_p\ . \tag{4.2}$$

[For a derivation, see José, et al., Ref (14).] The recursion relation for y is the same as in Sec. 2:

$$\frac{dy}{d\ell} = (2-\pi\tilde{K})\, h_p \quad . \tag{4.3}$$

The recursion relation for $\tilde{K}$ may be written

$$\frac{d\tilde{K}^{-1}}{d\ell} = \text{const } y^2 - \text{const } h_p{}^2 \quad . \tag{4.4}$$

The constants in (4.4) are positive, but their precise values are not important for our purposes.

Note that h_p decreases with increasing ℓ provided that

$$\tilde{K} < p^2/8\pi \quad . \tag{4.5}$$

Of course, y decreases with increasing ℓ provided that

$$\tilde{K} > 2/\pi \quad . \tag{4.6}$$

These two inequalities may be satisfied simultaneously, provided that $p > 4$.

For $p > 4$ we find in fact that there are two phase transitions.[14] At intermediate temperatures $T_{c1} < T < T_{c2}$ we find an X-Y-like phase where the correlation function for ψ has quasi-long range order

$$\langle\psi^*(r)\psi(0)\rangle \sim 1/r^\eta \quad . \tag{4.7}$$

The values of $h_p(\ell)$ and $y(\ell)$ both tend to 0 for large ℓ in this phase. The exponent η in (4.7) is related to the value of $\tilde{K}(\ell)$ in the same way as in Sec. 2. The inequalities (4.5) and (4.6) therefore give a restriction on the value of η

$$\frac{4}{p^2} \leq \eta \leq \frac{1}{4} \quad . \tag{4.8}$$

At high temperatures ($T > T_{c2}$) we find a "paramagnetic" phase where the

the order parameter ψ displays short-range order in the form of Eq. (2.9). The value of y becomes large for large ℓ in this region, while $\tilde{K}(\ell)$ tends to 0. At low temperatures ($T < T_{c1}$) we find that h_p becomes large for large ℓ. We interpret this as a "ferromagnetic" phase with true long-range order

$$<\psi> \neq 0 \quad . \tag{4.9}$$

In the vicinity of T_{c2} for $p > 4$, one finds according to Eq. (4.2) that h_p tends rapidly to 0 for large ℓ. One can then focus attention on the recursion relation for y and $\tilde{K}$. We say then that h_p is an irrelevant perturbation. The nature of the phase transition at T_{c2} is then exactly the same as in the ordinary X-Y model studied in Sec. 2, where h_p was set equal to 0 at the beginning.

In the neighborhood of T_{c1} we may set the variable $y = 0$. The recursion relations (4.2) and (4.4) are then identical to the recursion relation in Sec. 2, if we simply replace $\tilde{K}$ by $p^2/(16\pi^2\tilde{K})$. The phase transition is therefore mathematically equivalent to the phase transition in the X-Y model. In particular, the free energy and all its derivatives should be continuous at T_{c1}.[14]

For $p \leq 4$, there is no X-Y like intermediate phase, since (4.5) and (4.6) cannot be simultaneous satisfied. For p = 2, 3, and 4, we expect a direct transition from the ferromagnetic to the paramagnetic phase. The nature of that transition cannot be identified by the methods of the present paper. It is reasonable to assume that the critical exponents for p = 2 and p = 3 are determined by the symmetry of the system and are the same as for the Ising model and the 3-state Potts model respectively.[55] The case p = 4 probably has variable critical exponents.[14] For p = 1, there should be no phase transition, as the expectation value $<\psi>$ is different from 0 for all values to T.

The renormalization group analysis described above is not directly applicable to the case of strong h_p. On the basis of an approximate renormalization group analysis, using Migdal's techniques,[2] José, et al,[14] suggested that it is necessary to have $p \gtrsim 9$ for the X-Y like phase to occur in the discrete planar rotator model. More recent estimates suggest that a somewhat smaller value of p may be sufficient, as discussed in Prof. Suzuki's talk.[9,56] The analysis of the present section can, however, rule out the possibility of the existence of an X-Y like phase for $p < 4$, no matter how strong the interaction. For, if the X-Y like phase does exist, then the parameters $y(\ell)$ and h_p must flow to small values at long wavelengths, and therefore the analysis of this section applies.

If vortices are ruled out from the beginning, ($y(0) = 0$) then the X-Y model with cos $p\phi$ perturbations becomes equivalent to the so-called sine-Gordon model.[31,57] It follows from the recursion relations (4.2) and (4.4) that there is a single transition of the Kosterlitz-Thouless type, at a value of temperature where (4.5) becomes an equality. The sine-Gordon model in turn is a model for the so-called roughening transition that occurs on crystal surfaces in three dimensions.[57]

5. MELTING IN TWO DIMENSIONS

In this section, I wish to discuss a theory of melting in two dimensions, based on the assumption that the melting occurs by unbinding of pairs of dislocations, analogous to the unbinding of vortex pairs at the superfluid transition.[58] The theory which is based on the ideas of Kosterlitz and Thouless,[4-6] was worked out by D.R. Nelson and myself.[15-17] A number of the results were obtained independently by A.P. Young.[18]

I shall restrict myself here to the melting of a triangular lattice on a smooth substrate. The theory should be directly applicable to the melting of the two-dimensional solid formed at low temperatures by electrons trapped on a liquid helium surface.[59] Other possible applications include phase transitions in free suspended smectic liquid-crystal films[60] and possible phase transition in lipid layers floating on water. The theory has also been applied recently to the melting of a vortex lattice in a thin-film superconductor in an external magnetic field.[61] With some modifications, the theory may also describe melting on an incommensurate crystalline substrate.[15] (Examples here are transitions in adsorbed gas layers on substrates such as graphite.[62]) The theory may also be applicable to reconstructed surfaces without any adsorbate present when there is a surface periodicity incommensurate with the periodicity of the bulk lattice. The theory of two dimensional melting may also be an appropriate starting point for an understanding of phase transitions in certain bulk smectic phases if the coupling between the layers in the smectic is sufficiently weak.[63-65] (See Sec. 6C, below.)

A. Analogy to the superfluid.

As I have already suggested, there is a strong analogy between the theory of two-dimensional melting and the theory of superfluid transition in two dimensions. The quantity analogous to the local phase $\phi(\vec{r})$ in the superfluid or X-Y model, is the vector field $\vec{u}(\vec{r})$ measuring the displacement of atoms from their equilibrium positions in the solid. Analogous to the local superfluid velocity, $v_s=\vec{\nabla}\phi$, will be the local strain field, defined as the symmetric derivative of the displacement

$$u_{ij} = \tfrac{1}{2}(\partial_i u_j + \partial_j u_i) \ . \qquad (5.1)$$

(The indices i and j here refer to the Cartesian coordinates x, y.)

The fact that the displacement is a vector quantity rather than scalar will of course lead to certain complications not present in superfluid case. Analogous to the superfluid density ρ_s there are now two elastic constants, the Lamé coefficients, μ and λ. Corresponding to the bare Hamiltonian (2.13), we now have the bare elastic Hamiltonian[66]

$$H_0 = \tfrac{1}{2}\int d^2r \ [2\mu_0 u_{ij}u_{ij} + \lambda_0 u_{ii}{}^2] \ . \qquad (5.2)$$

The constants μ_0 and λ_0 are the bare values of the Lamé coefficients, and we have used a summation convention for repeated indices in (5.2).

The order parameter for the superfluid or X-Y model was given, in the absence of magnitude fluctuation, by $e^{i\phi(\vec{r})}$. In the solid, we define a translational order parameter $\rho_{\vec{G}}$ for each reciprocal lattice vector $\vec{G}$ of the crystal by

$$\rho_{\vec{G}}(\vec{r}) \equiv e^{i\vec{G}\cdot\vec{u}(\vec{r})} \ . \qquad (5.3)$$

As observed by Landau and by Peierls in the 1930's, the mean square displacement of a two-dimensional solid is expected to diverge logarithmically due to the effect of thermal excitation of long wave length vibrational modes.[1] In analogy to Eq. (2.18), one expects a power-law fall-off of the correlation function for the translational order parameter at large separation r (quasi-long range order) given by[3]

$$<\rho_{\vec{G}}(\vec{r})^* \ \rho_{\vec{G}}(0)> \sim (\tfrac{1}{r})^{\eta_G} \ , \qquad (5.4)$$

where the exponent $\eta_{\vec{G}}$ is related to the elastic constants by

$$\eta_{\vec{G}} = \frac{|G|^2 T}{4\pi\mu} \frac{(3\mu+\lambda)}{(2\mu+\lambda)} \quad . \tag{5.5}$$

The quasi-long-range translation order is reflected in the behavior of the x-ray structure factor $S(\vec{q})$ defined by

$$S(\vec{q}) \equiv \langle|\rho(\vec{q})|^2\rangle \quad , \tag{5.6}$$

where $\rho(\vec{q})$ is the Fourier transform of the density. Specifically, one finds a set of singularities at wave vectors equal to the reciprocal lattice vectors $\vec{G}$ of the form

$$S(\vec{q}) \sim \sum_{\vec{G}} |\vec{q}-\vec{G}|^{-2+\eta_G} \tag{5.7}$$

These power law singularities replace the δ-function Bragg peaks and phonon side bands which occur in three dimensions.

In addition to broken translational symmetry, a crystal is characterized by broken orientational symmetry. We may define an orientational order parameter for hexagonal crystal by

$$\psi(\vec{r}) = e^{6i\theta(\vec{r})} \quad , \tag{5.8}$$

where $\theta(\vec{r})$ an angle describing the orientation of a nearest-neighbor bond at point $\vec{r}$. In a perfect crystal at $T = 0$, and angle θ is the same for all bonds, modulo 60°. Then ψ is independent of $\vec{r}$; and

$$\langle\psi^*(\vec{r})\psi(0)\rangle = 1 \quad . \tag{5.9}$$

Unlike the mean square displacement, the expectation value $\langle\theta^2\rangle$ remains finite at $T \neq 0$, even in two dimensions.[67] There is therefore true long-range order for the orientational parameter ψ:

$$\lim_{r \to \infty} \langle \psi^*(\vec{r})\, \psi(0) \rangle = \text{const} > 0 \quad . \tag{5.10}$$

For long wavelength fluctuations, the angle θ is related to the displacement field by

$$\theta = \tfrac{1}{2}\vec{\nabla} \times \vec{u} \tag{5.11}$$

In Fourier transform we see that $|\theta(\vec{k})|^2$ is proportional to $k^2|\vec{u}(\vec{k})|^2$. The extra factor of k^2 removes the divergence arising from the long wavelength phonon modes, which is the reason that $\langle\theta^2\rangle$ is finite.

B. Dislocations in two dimensions.

A dislocation in a two-dimensional crystal is a point defect analogous to a vortex in the superfluid. When a dislocation is present, it is no longer possible to define a single-valued continuous displacement $\vec{u}(\vec{r})$. The strength of the dislocation is characterized by a Burgers vector $\vec{b}$, defined by[68]

$$\int_C \frac{\partial u_i}{\partial \vec{r}} \cdot d\vec{r} = b_i \tag{5.12}$$

where the contour C encircles the dislocation. Since the displacement $\vec{u}$ is uniquely defined modulo a vector on the Bravais lattice of the crystal, the Burgers vector $\vec{b}$ must itself be a vector on the Bravais lattice. Except at the dislocation core, the order parameters $\rho_{\vec{G}}(\vec{r})$ remain single-valued and continuous since

$$e^{i\vec{G}\cdot\vec{b}} = 1 \quad . \tag{5.13}$$

For present purposes, we need only consider elementary dislocations, where $\vec{b}$ has its minimum allowed value b_0, equal to the lattice constant. There are six possible orientations for the elementary Burgers vector of a triangle lattice.

In Fig.(6a) we have illustrated the elementary dislocation for a square lattice, where the dislocation may be thought of as simply the termination of an extra half-row of atoms. We have also illustrated a geometric construc-

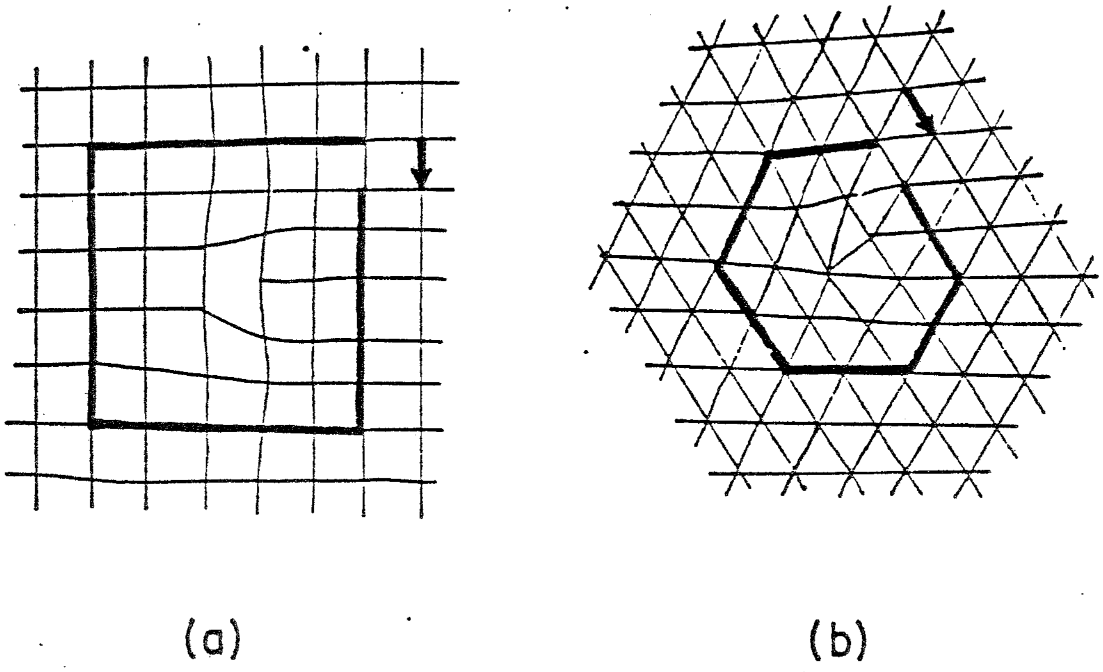


Fig. 7. Elementary dislocations in (a) a square and (b) a triangle lattice. Heavy lines are contours that would be closed if the dislocation were not present. Burgers vector indicated by arrow, is the amount by which the contour fails to close.

tion for determining the Burgers vector. The corresponding figure for a triangle lattice is illustrated in Fig (7b).

From Eq. (5.12) it is reasonable to guess that the strain field in the neighborhood of a dislocation will fall off as 1/r, and that the energy of an isolated dislocation will diverge as the logarithm of the size of the system. Then, for a dislocation pair, with equal and opposite Burgers vectors,

$$\vec{b}_1 = -\vec{b}_2 \equiv \vec{b} \quad , \tag{5.14}$$

one would expect to find a finite energy proportional to the logarithm of the separation. The result obtained from elasticity theory, in fact, is that the energy of a pair at large separation $\vec{r}$ is given by[68]

$$E_2(\vec{r}) = \overline{K}\ [\ln(\frac{r}{a}) - \frac{(\vec{b}\cdot\vec{r})^2}{b^2r^2}\ ] + 2E_c \quad , \tag{5.15}$$

where E_c is the dislocation core energy and $\overline{K}$ is related to the elastic constants by

$$K = \frac{b^2}{\pi}\frac{\mu(\mu+\lambda)}{(2\mu+\lambda)} \quad . \tag{5.16}$$

Note the presence of the second term on the right-hand side of (5.15), which depends on the angle between the Burgers vector $\vec{b}$ and separation r. The energy of an isolated dislocation is given by

$$E_1 = \tfrac{1}{2}\bar{K}\,\ln(R/a) \tag{5.17}$$

where R is the radius of the system. Unfortunately, the equations of elasticity are considerably more complicated than the equations of electrostatics, and we shall not be able to give a derivation of these results here.

If the dislocation pair $\vec{b}_1$ and $\vec{b}_2$ are the only dislocations present in the system, then the elastic constants μ and λ entering (5.16) should be interpreted as the "bare elastic constants" μ_0 and λ_0, which are renormalized from their T = 0 values only by the presence of non-linear phonon interactions in the system. We are ultimately interested, however, in the free energy of an isolated dislocation, or the free energy of a dislocation pair at large separation, *in the presence of a finite density of bound dislocation pairs*, which will occur in thermal equilibrium even in the solid phase. We may use Eqs. (5.15)-(5.17), for this purpose, provided that we interpret the elastic constants μ and λ in (5.1) to mean the macroscopic renormalized elastic constants μ_R and λ_R.

Comparing Eq. (5.17) with Eq. (2.51), we may immediately write down the Kosterlitz-Thouless criterion for stability of a solid phase against the formation of an isolated dislocation:

$$\bar{K}_R/T \geq 4 \quad . \tag{5.18}$$

The Kosterlitz-Thouless theory of melting and the renormalization group calculation described below will apply if inequality (5.18) becomes an equality at the melting transition T_m:

$$\lim_{T\to T_m} \bar{K}_R/T = 4 \tag{5.19}$$

Note that the combination of elastic constants entering Eq. (5.16) is not the same as the combination entering (5.5). The value at melting of the exponent η_G is therefore not a universal quantity.

C. Renormalization equations.

Our first task, then, is to study the renormalization of the elastic constants μ and λ. In the presence of a stress field σ_{ij}, there will be a "force" on a dislocation given by [68]

$$f_i = \varepsilon_{ji}\sigma_{j\ell}b_\ell \quad , \tag{5.20}$$

where ε_{ji} is the unit antisymmetric tensor. This force will tend to cause the dislocation to move in a direction such as to relax the stress. Bound dislocation pairs will be polarized by an applied stress, and the resulting polarization will lead to a finite reduction in the elastic constants μ and λ. If free dislocations are present, however, they will continue to flow as long as stress is applied and the polarization will increase without limits. The system can no longer sustain a sheer stress in equilibrium, and melting has occured.[68]

In analogy with our calculations in Sec. 2, we would like to define partially renormalized elastic constants $\mu(\ell)$ and $\lambda(\ell)$, where we have taken into account the polarizability only of pairs which are separated by a distance r', such that

$$r' < r \equiv a_0 e^\ell \quad . \tag{5.21}$$

We define an elastic constant $\overline{K}(\ell)$ which is related to $\mu(\ell)$ and $\lambda(\ell)$ by Eq. (5.14), and we define a reduced elastic constant $K(\ell)$ by

$$K(\ell) = \overline{K}(\ell)/T \quad . \tag{5.22}$$

We define a dislocation fugacity $y(\ell)$ analogous to the fugacity of the vortices in Sec. 2.

The recursion relations for $\mu(\ell)$ and $\lambda(\ell)$, and hence for $\overline{K}(\ell)$ are similar to those in Sec. 2. If we define a variable, x, by

$$2x \equiv \left(2-\frac{K}{8\pi}\right) \quad , \tag{5.23}$$

then the recursion relation for x has the form

$$\frac{dx}{d\ell} = \tfrac{1}{2}Ay^2 + O(y^3) \quad , \tag{5.24}$$

where

$$A = 3\pi e^{-2}\ [2I_0(2) + I_1(2)] \quad . \tag{5.25}$$

The Bessel functions I_0 and I_1 arise from the integration over the angle between the separation vector $\vec{r}$ and the Burgers vector $\vec{b}$. A new feature of (5.24) which did not occur in Eq. (2.94) is that the correction to the leading term is of order y^3. This occurs because it is now possible to have a neutral triplet of elementary dislocations, in which the Burgers vectors are oriented 120° apart from each other, and the sum of the Burgers vectors is equal to 0. The energy of such a triplet is seen to be finite, and the number-density of triplets will be proportional to y^3.

In the region of interest (x and y small) the recursion relation for y may be written

$$\frac{dy}{d\ell} = 2xy + By^2 + O(y^3) \tag{5.26}$$

where

$$B = 2\pi e^{-1}\ I_0(1) \quad . \tag{5.27}$$

The first term on the right-hand side of (5.26) is identical to the corresponding term in Eq. (2.98), and arises from the same physical effects, namely from the geometric redefinition of the length scale and from the work necessary to increase the separation of the pair by an amount $d\ell$. The term By^2 is new, and arises from the appearance of two dislocations whose Burgers vectors b_1 and b_2 differ by 120° and whose spatial separation r falls in the range

$$a_0 e^{\ell} < r < a_0 e^{\ell+\delta\ell} \quad . \tag{5.28}$$

Our renormalization procedure is defined such that when we increase our length scale by the fraction $\delta\ell$, the two Burgers vectors are replaced by a single dislocation whose Burgess vector is the sum of $\vec{b}_1$ and $\vec{b}_2$ and whose position is midway between the positions of the two dislocations. Clearly, this will give a contribution to $y(\ell+\delta\ell)$ which is of the order $y(\ell)^2$.

D. Results

The recursion relations (5.26) and (5.24) may be analyzed in a manner similar to the Kosterlitz recursion relations of Sec. 2. The flow diagram is qualitatively the same as in Fig. 5. For temperatures at or below the melting temperature T_m, we find for large ℓ that

$$y(\ell) \to 0 \quad . \tag{5.29}$$

The renormalized elastic constants μ_R and λ_R are finite for $T \leq T_m$ and the limiting value of $\overline{K}_R$ obeys Eq. (5.17). In limits $T \to T_m$ from below, we find

$$\mu_R = \mu_c + \text{const}\ (T_m-T)^{\overline{\nu}} \tag{5.30}$$

$$\overline{\nu} = .36963.... \tag{5.31}$$

The difference from the behavior in the case of the planar spin model ($\overline{\nu} = \frac{1}{2}$) arises from the term By^2 in (5.24).

For T just above T_m the fugacity $y(\ell)$ at first decreases with increasing ℓ and then begins to increase. When $y(\ell)$ comes of order unity, we can no longer use our recursion relation, and we must simply make the assumption that the remaining dislocations are essentially free, i.e., that they behave like a weakly-interacting plasma. We argue that the translational correlation functions show short-range order for $T>T_m$

$$<\rho_{\vec{G}}(\vec{r})^* \rho_{\vec{G}}(o)> \sim e^{-r/\xi} \tag{5.32}$$

where ξ is equal to the mean distance between free dislocations. A solution of the recursion relations (5.26) and (5.24) yields

$$\xi \approx \left(\frac{1}{n_{free}}\right)^{\frac{1}{2}} \propto \exp\left(\frac{b}{T-T_m}\right)^{\bar{\nu}} \qquad (5.33)$$

where $\bar{\nu}$ is again given by (5.31).

Since relaxation of a shear stress is caused by the motion of free dislocations, we expect that the viscosity will be inversely proportional to the density n_{free}. Thus, as T approaches T_m from above the viscosity should diverge proportional to ξ^2. (We neglect here the very weak logarithmic divergence of the viscosity at long wave lengths due to the effects of mode coupling and the long-time tails in two dimensions.[69])

E. The hexatic phase.

Our most interesting result concerns the behavior of the order parameter for bond orientation $\psi = e^{6i\theta}$, above T_m.

In contrast to the short-range order that one would expect for an isotropic fluid, we find the result that for temperatures just above T_m,

$$<\psi^*(\vec{r})\psi(0)> \sim (1/r)^{\eta_\psi} \qquad (5.34)$$

Thus there is a quasi-long range order in the orientation of the bonds, which reflects a term in the free energy of the form

$$\delta F = \tfrac{1}{2}\int K_A|\nabla\theta|^2\, d^2r \; . \qquad (5.35)$$

The exponent η_ψ in (5.34) is given by

$$\eta_\psi = \frac{18T}{\pi K_A} \quad . \qquad (5.36)$$

[This equation differs by a factor 36 from the corresponding equation for the X-Y model (2.53), because of the occurrence of the quantity 6θ in the definition of the order parameter (5.8).

A system with the properties just described is a new type of liquid crystal, which we have termed the <u>hexatic phase</u>. The constant K_A is a Frank elastic constant for the liquid crystal. It is found that K_A diverges as T approaches T_m, according to

$$K_A \propto \xi^2 \to \infty \text{ for } T \to T_m^{\;+} \tag{5.37}$$

Although a mathematical derivation of the results (5.34)-(5.37) will be given below, their physical origin may be understood by examining Fig. 7. It will be seen that dislocations are much more effective in destroying translational order than they are in destroying orientational order. In particular, the translational order parameters $\rho_{\vec{G}}$ are 180° out of phase between one side of the dislocation and the other, but the bond orientations are only perturbed in the immediate vicinity of the dislocation core. Thus, it is not surprising that some kind of orientational order can persist with a small density of free dislocations present.

If the system just above T_m has the liquid-crystal properties described above, then a phase transition to the isotropic fluid phase must occur at some higher temperature T_i, as indicated in Fig. 8.

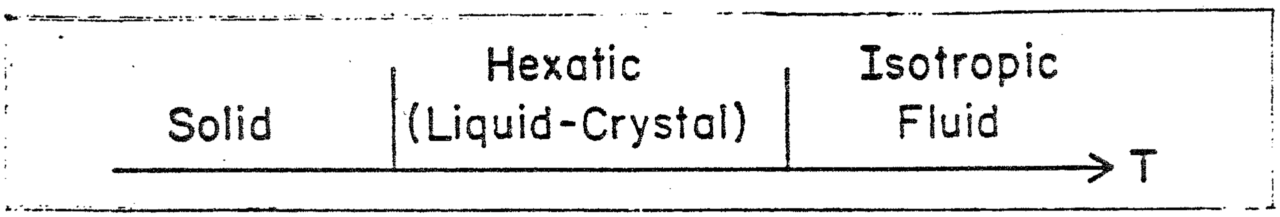


Fig. 8. Phase diagram obtained from the dislocation theory of melting of a two-dimensional solid.

The proposed mechanism for the transition to the isotropic phase is the appearance above T_i of another kind of topological defect known as a <u>disclination</u>. An elementary disclination in the hexatic phase is illustrated in Fig. 9a. Note that the bond-orientation angle θ changes by 60° as one moves along a contour which encircles the disclination. For comparison, we show Fig. 9b the elementary disclination in a nematic liquid crystal. Here the order parameter refers to the orientation of the axis of a long molecule, and the elementary disclination involves a rotation of 180°.

The energy of a set of disclinations in the hexatic phase may be calculated in the same manner as the energy of vortices in the superfluid. Because the elementary disclination has a strength of 60°, however, the angular distortions are six times smaller than in the superfluid case, and the free energies are smaller by a factor of 36. The free energy of a pair of disclinations with

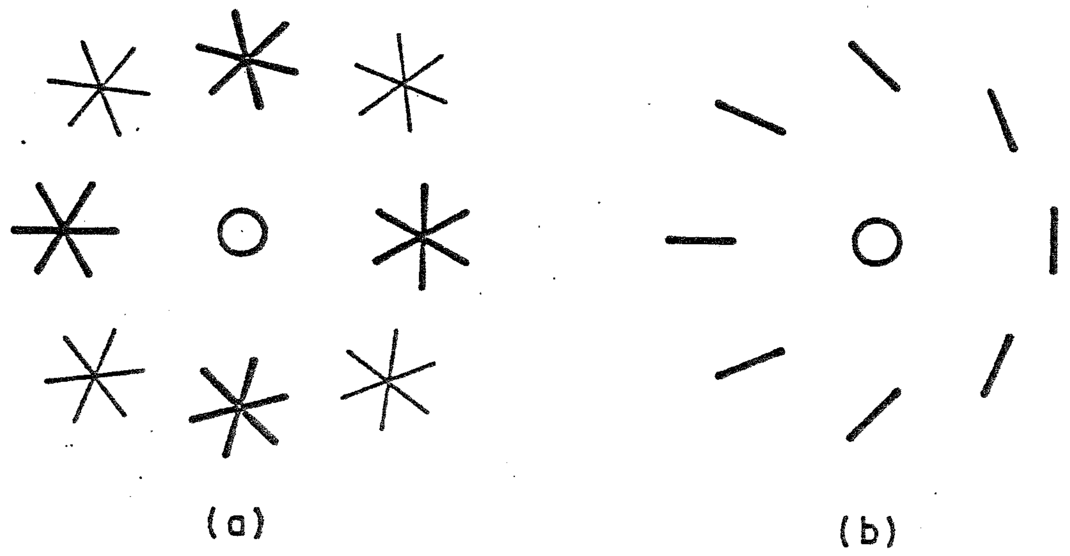


Fig. 9. Elementary disclinations, (a) in a hexatic and (b) in a two-dimensional nematic liquid crystal. Six-pointed stars in (a) show the orientation of the nearest-neighbor bonds, in various regions of space. Lines in (b) show orientation of molecular axis. Only one sign of disclination is shown.

separation r is given by

$$\delta F \approx \frac{\pi}{18} K_A \ln r \quad . \tag{5.38}$$

The Kosterlitz-Thouless criterion for the stability of the hexatic phase against the formation of free disclinations may then be written

$$K_A \leq 72T/\pi \quad , \tag{5.39a}$$

or using (5.36)^{70}

$$\eta_\psi \leq \tfrac{1}{4} \quad . \tag{5.39b}$$

The renormalization gorup analysis of Sec. 2 may be applied with trivial modifications, to the phase transition at T_i and, of course, we find a phase transition of the Kosterlitz-Thouless type.

We may summarize the occurrence of topological defects as follows: Dislocations which are free in the isotropic fluid and hexatic phases can occur in the solid only as neutral bound states whose energy is proportional to the logarithm of the separation. Disclinations which are free in the isotropic phase can occur in the hexatic only in bound pairs $E \propto \ln r$. It is interesting to note that a dislocation may be regarded as a tightly bound pair of disclinations with the Burgers vector of the dislocation determined by the separation of the disclinations.[68] Thus we may say that disclinations may occur in equilibrium in the solid, provided they are bound in quartets with no net dipole moment. The energy of the group is very large, however, ($E \propto r^2$) if the four disclinations are not grouped into pairs.

If the renormalization group theory is correct, the phase transitions at T_m and T_i should not be apparent in the free energy or its derivatives. As in the case of the superfluid, one predicts that the free energy and all of its derivatives should be continuous at these phase transitions. In order to see the transition, one must study properties such as the elastic constants which vanish discontinuously at T_m, or the Frank constant which vanishes discontinuously at T_i. Alternatively, one may be able to observe the change in character of the long wavelength behavior of the correlation functions at the transition.

It should be emphasized again that a renormalization group analysis is only exact when the length scale of interest is large compared to the lattice spacing. If a critical point transition occurs, then large length scale fluctuations are crucial; the renormalization group can give us some important consistency tests and can tell us the nature of the critical point when it occurs. Our analysis cannot rule out, however, the possibility of a phase transition arising from a mechanism very different from the one considered, and in particular, we cannot rule out the possibility of a first order transition determined by processes on the scale of one or two lattice constants. In fact, we cannot rule out the possibility that there may be, in any particular solid, a large first-order transition which carries one directly from the solid to the isotropic fluid phase. Our analysis does guarantee, however, that if the Kosterlitz-Thouless mechnism applies, so that melting occurs by the appearance of a small density of free dislocations, then two transitions are necessary before isotropic fluid is reached.

F. Methods for calculating orientational fluctuations, $T>T_m$.

The results (5.34) to (5.37) are derived by analysis of fluctuations in the bond angle field θ. The angle θ is realted to the displacement by Eq. (5.1). By using the known solutions for the displacement field caused by a dislocation [68], one may derive the relation

$$\theta(\vec{r}) = \frac{-1}{\pi} \int \frac{\vec{b}(\vec{r}')\cdot(\vec{r}-\vec{r}')}{\left|\vec{r}-\vec{r}'\right|^2}\, d^2r' \tag{5.40}$$

where $\vec{b}(\vec{r}')$ is the Burgers-vector density at point r'. Taking the Fourier transform of (5.38), we find

$$\hat{\theta}(\vec{q}) = -q_j\, \hat{b}_j(\vec{q}) \,/\, q^2 \tag{5.41}$$

$$<|\theta(\vec{q})|^2> = \frac{q_i q_j}{q^4} <\hat{b}_i(\vec{q})\hat{b}_j(-\vec{q})> \tag{5.42}$$

(In these equations, a hat has been used to indicate Fourier transformed quantities). If Eq. (5.35) is correct, then the correlation function (5.42) should have the form at long wavelength:

$$<|\hat{\theta}(q)|^2> = \frac{k_B T}{K_A q^2} \tag{5.43}$$

Any dislocations which are bound in neutral pairs or triplets will give a contribution to $<\hat{b}_i(\vec{q})\hat{b}_j(-\vec{q})>$ which vanishes in the limit $q \to 0$, and therefore bound dislocations will not contribute to the term exhibited in (5.43). The contribution of the free dislocations may be estimated by using an effective Hamiltonian

$$\mathrm{Heff} = \frac{K}{2b_0{}^2} \sum_{\ell \neq \ell} \left[-\vec{b}_\ell \cdot \vec{b}_{\ell'} \ln\left|\frac{\vec{R}_\ell - \vec{R}_\ell}{a}\right| + \frac{(\vec{R}_\ell - \vec{R}_{\ell'})\cdot\vec{b}_{\ell'}\ (\vec{R}_\ell - \vec{R}_{\ell'})\cdot\vec{b}_{\ell'}}{b^2 |\vec{R}_\ell - \vec{R}_{\ell'}|^2} \right] \tag{5.44}$$

where the sum is over a density n_{free} of free dislocations and the elastic constant $\overline{K}$ is renormalized by the polarizability of the bound pairs. Equation (5.44) may be written in Fourier transform as

$$H_{eff} = \tfrac{1}{2} \sum_{\vec{q}} \hat{b}_i(\vec{q})\hat{b}_j(-\vec{q}) \left| \frac{K}{b_0^2 q^2} \left(\delta_{ij} - \frac{q_i q_j}{|q|^2}\right) \right| \qquad (5.45)$$

According to (5.45), there is a large cost in potential energy proportional to $1/q^2$ associated with transverse fluctuations in the Burgers vector density $\vec{b}$. There is no such cost for longitudinal fluctuations and we expect that the longitudinal part of $\langle b_i(\vec{q})b_j(-\vec{q})\rangle$ is finite at q-0, and or order $b_0{}^2 n_{free}$. We therefore estimate, using (5.42) and (5.43) that

$$\frac{K_A}{k_B T} \approx \frac{1}{b_0{}^2 n_{free}} \approx \frac{\xi^2}{b_0{}^2} \qquad (5.46)$$

G. Application to the two-dimensional electron solid.

At this point, one may ask whether there is any evidence that the dislocation theory of melting is correct in any achievable two-dimensional system. There is at least some supporting evidence from computer simulations of two-dimensional systems. Frenkel and McTague have analyzed numberical data for a system of particles interacting with a Lénard-Jones 6-12 potential in two-dimensions, and have found what appears to be a hexatic phase over a considerable range of temperature above T_m.[71,72] There is also some evidence that melting of the two-dimensional electron system may be consistent with the Kosterlitz-Thouless-Halperin-Nelson-Young theory.

The temperature of classical two-dimensional electron system is measured by the dimensionless parameter[73]

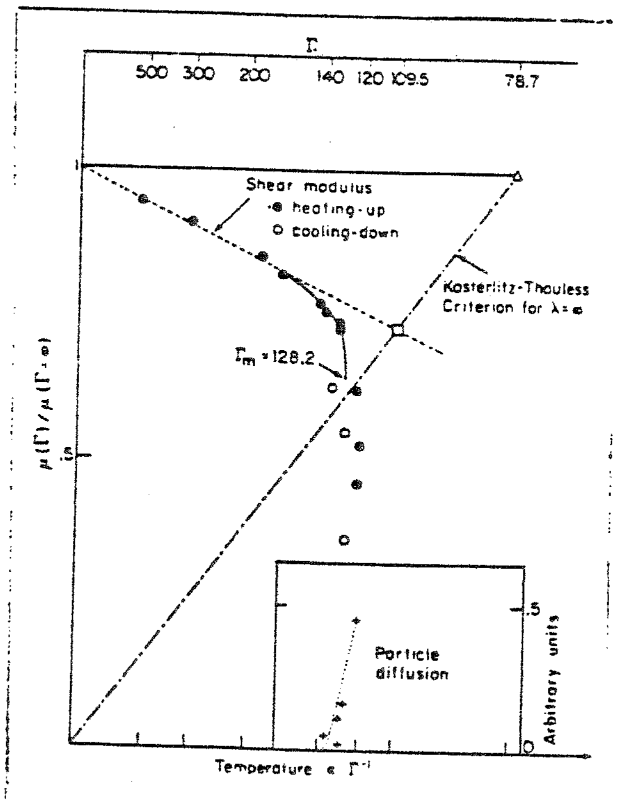
$$\Gamma^{-1} = \frac{T}{e^2 \pi^{\frac{1}{2}} n} \qquad (5.47)$$

where e is the electronic charge and n is the number of electrons per unit area. The denominator in (5.47) is just the Coulomb energy of a pair of electrons at a separation equal to the radius of the Wigner-Seitz cell. Small values of Γ correspond to high temperatures, or a weakly-coupled plasma, while values of Γ in the range $1<\Gamma<100$ represent a strongly coupled plasma. Some place in the range $\Gamma \gtrsim 100$ we expect the transition to a two-dimensional Wigner crystal. Experimental observations of[9] two-dimensional solid formed by electrons on the surface of liquid helium, by Grimes & Adams,[59] are consistent with a melting temperature in the range $\Gamma_m = 131\pm7$. Estimates of Gann, et al.,[74] based on Monte Carlo simulations, give the result $\Gamma_m \approx 125$, consistent with these experiments, although earlier computer simulations by Hockney and Brown[75] gave a higher melting temperature, $\Gamma_m = 95$.

A theoretical estimate of the melting temperature of the two-dimensional electron lattice was provided by Thouless.[76] Using the known values of μ and λ, at T=0 in the Kosterlitz-Thouless cirterion, Eq. (5.17), Thouless obtained the estimate $\Gamma_m = 78.7$. (The bare value of λ is infinite for the Coulomb system so that the melting temperature is determined by μ in this approximation.)

The Thouless estimate differs considerably from the experimental value $\Gamma_m \approx 130$, and it is important to know whether renormalization of the elastic moduli can account for this difference. In order to investigate this question, Rudolph Morf[77] has undertaken a molecular dynamics calculation of the shear modulus in the solid phase of the two-dimensional electron solid. The results are illustrated in Fig. 10.

Fig. 10. Temperature dependence of shear modulus μ in the 2-D electron solid. (From R.H. Morf.[77]) The circles represent the computer-simulation results for $\mu(\Gamma)/\mu(\Gamma=\infty)$ as function of the dimensionless temperature Γ^{-1}. The values shown as full circles are obtained on heating; the open circles are obtained on cooling-down from $\Gamma = 120$. The solid curve, ending at $\Gamma_m = 128.2$ displays the results of a renormalization group calculation, in which the starting value μ_0 of shear modulus was taken from a linear extrapolation of the low temperature results (dashed line). For comparison, we show the Thouless value $\Gamma = 78.71$ obtained by neglecting all renormalization effects. Also shown, in inset (dotted line and +), is a measure of the observed particle diffusion which rises sharply at $\Gamma \approx 130$.



For temperatures up to approximately 3/4 of the melting temperature, Morf found a linear decrease in the shear modulus which he attributed to the effects of nonlinear interaction among the phonons. This temperature dependence is indicated by the dashed line in Fig 10. The further effects of dislocation polarizability could be estimated using the phonon-renormalized shear modulus as the starting value μ_0. The phonon interactions do not affect the starting value of λ ($\lambda_0 = \infty$), although the final value of λ_R will be finite due to the effects of interstitials and vacancies. The starting value of the dislocation fugacity y_0 was obtained from the numerical results of Fisher, Halperin and Morf[78] for the dislocation core energy E_c using the crude assumption that the core free energy at finite temperatures is reduced from the T=0 value in proportion to the reduction of the bare shear modulus μ_0 due to phonon interactions.

The resulting prediction for the macroscopic shear modulus μ_R is shown as the solid curve in Fig. 10. The predicted value of $\Gamma_m = 128.2$ is in good agreement with the experimental results.

Very recently, D.S. Fisher has calculated analytically the first correction to the shear modulus fo the classical 2-D electron solid arising from non-linear phonon interactions, at low temperatures. (D.S. Fisher, private communication.) The results agree with the molecular dynamic results (dotted line in Fig. 10).

6. LIQUID CRYSTAL FILMS WITH TILTED MOLECULES

In recent years, techniques have been developed for growing very thin films of smectic liquid crystals.[79] Films as thin as two molecular layers have been grown and stable films of one molecular layer may be possible in some cases. A variety of phase transitions occurs in such films, and they offer interesting possibilities for the investigation of two-dimensional phase transitions.[60,79]

The smectic liquid crystals are generally formed from long organic molecules. For our purposes, we may consider these molecules to be rods, indistinguishable at the two ends. In many cases, the rods tend to orient perpendicular to the plane of layers (e.g., smectic A and smectic B phases).[63] When the molecules order within a layer in such a case they tend to form a regular triangular lattice and the theory of melting discussed in the previous section should apply. In other cases, the molecular axes are tilted relative to the normal to the plane and there is a tendency for the axes of different melecules to point in the same direction and to order at low temperatures.[63,79] The tilted molecules may also tend to form a regular solid array within the plane at low temperatures, and it is interesting to investigate the phases that can occur when the order parameter for molecular tilt orientation is coupled to the translational order parameters $\rho_{\vec{G}}$ and to the order parameter for bond orientation ψ, discussed in the previous section. Such an investigation has been carried out recently by David Nelson and myself.[19] I present here only a few of the results.

A. Fluid phases.

Let us describe the orientation of a molecule by unit vector $\hat{n}$, and let us introduce a tilt orientation order parameter

$$\Phi \equiv n_x + in_y \equiv (\sin\gamma)\, e^{i\phi} \quad , \tag{6.1}$$

where the x and y directions are in the plane of the film. Although the orientations $\hat{n}$ and $-\hat{n}$ are indistinguishable, the sign of Φ is determined and is meaningful if we adopt the convention that $n_z > 0$. [The hypothetical case $n_z = 0$, corresponding to a two-dimensional "nematic", is different, because Φ and $-\Phi$ are equivalent in that case.]

Couplings between the bond-orientation and tilt degrees of freedom lead to a rich variety of possible phases and phase diagrams. Tilted and untilted versions of the hexatic and liquid phases may be understood in terms of an effective Hamiltonian functional of the bond orientation $\theta(\vec{r})$ and tilt orientation field $\phi(\vec{r})$, namely

$$\frac{H}{k_B T} = \tfrac{1}{2}\int d^2r\,[K_6|\vec{\nabla}\theta|^2 + K_1|\vec{\nabla}\phi|^2 + 2g(\vec{\nabla}\theta)\cdot(\vec{\nabla}\phi)]$$

$$- h\int d^2r\, \cos[6(\theta-\phi)] \tag{6.2}$$

The quantity K_1 is a stiffness constant for fluctuations in the tilt orientations while K_6 is the Frank constant for fluctuations in the bond orientation.[80,81] The term proportional to h occurs because both $\theta(\vec{r})$ and $\phi(\vec{r})$ feel a six-fold symmetric potential when rotated with the other field held fixed. The gradient cross-coupling, proportional to g, is generated by the renormalization group even if it is initially absent. "Vortices" in the tilt orientation field $\phi(r)$ and "disclinations" in the bond orientation $\theta(\vec{r})$ are also taken into account. These excitations renormalize the elastic constants at large distances, and can also drive phase transitons by unbinding from a state consisting of tightly bound pairs. The "bare" constants in (6.2) will themselves have an analytic dependence on temperature due to the effects of fluctuations on the atomic length scale.

The Hamiltonian (6.2) may be treated by renormalization group methods similar to those discussed in the earlier parts of these lectures. The coupling h in (6.2) plays a role similar to the coefficient h_p of the cos $p\phi$ perturbation in Sec. 4.

The constant K_6 in (6.2) is related to the Frank constant K_A of Sec. 5 by $K_6 = K_A/k_BT$. The subscripts 6 and 1, which we use here to indicate quantities referring to the angles θ and ϕ respectively, were chosen because the bond orientation θ is defined modulo $2\pi/6$, while the tilt orientation ϕ is defined on the entire range from 0 to 2π.

A variety of possible phases follow from this model, which may be distinguished by the large distance behavior of the correlation functions

$$C_6(\vec{r}) \equiv \left\langle e^{6i[\theta(\vec{r}) - \theta(\vec{0})]} \right\rangle \tag{6.3}$$

$$C_1(\vec{r}) \equiv \left\langle e^{i[\phi(\vec{r}) - \phi(0)]} \right\rangle \ . \tag{6.4}$$

One possible phase diagram is shown schematically in Fig. 11, as a function of the inverse "bare" Frank constants K_1^{-1} and K_6^{-1}, with g and h small and fixed. The quantities K_1^{-1} and K_6^{-1} should both be monotonically increasing functions of temperature, so that a given material will trace a path from lower left to upper right in the figure, as temperature is increased. The solid phases shown in this diagram, in which $K_6=\infty$, will be discussed later.

Four fluid phases are indicated in the diagram, labelled A, A*, C, and C*. Phase A* is identical to the hexatic phase of Sec. 5, with short-range order in $C_1(\vec{r})$ and quasi-long-range order in $C_6(\vec{r})$.

Phase A, is an isotropic liquid phase, where both $C_1(\vec{r})$ and $C_6(\vec{r})$ decay exponentially at large r. The remaining fluid phases, C and C*, have quasi-long range order for both tilt and bond orientations; i.e., for large r we have

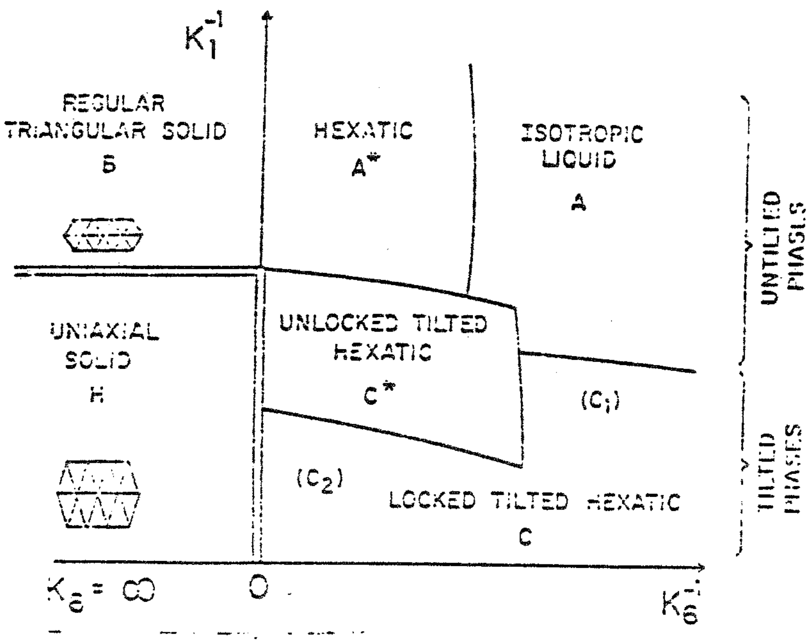


Fig. 11. Phase diagram for smectic liquid crystal layers, as a function of the inverse "bare" Frank elastic coefficients $K_1^{-1}(T)$ and $K_6^{-1}(T)$. Both solid and fluid phases are shown, and these can be either tilted or untilted. The Frank constant K_6 is infinite in the solid phases. Experiments with varying temperature might trace a path from the lower left to the upper right portion of the Figure, with increasing temperatures.

$$C_6(\vec{r}) \sim r^{-\eta_6(T)} \tag{6.5}$$

$$C_1(\vec{r}) \sim r^{-\eta_1(T)} \tag{6.6}$$

Phase C is a "locked" tilted hexatic phase in which long wavelength fluctuations in ϕ are tied to fluctuations in θ. The phase is characterized by a single renormalized (i.e., macroscopic) Frank constant K_+^R which describes the increase in energy caused by equal gradients in θ and ϕ. (Roughly one has $K_+^R = K_1+K_6+2g$). In this phase, the exponents η_1 and η_6 are related by

$$\eta_6 = 36\eta_1 = \frac{18}{\pi}\frac{k_BT}{K_+^R} \quad . \tag{6.7}$$

Phase C* is an "unlocked" tilted hexatic phase, in which long wave length fluctuations in ϕ and θ are independent. This phase has three renormalized Frank constants, K_1^R, K_6^R, and g_R, corresponding to the bare constants in (1.1), and there is no simple relation between η_1 and η_6:

$$\eta_6 = \frac{18K_1^R}{(K_6^R\, K_1^R - g_R{}^2)} \quad , \tag{6.8}$$

$$\eta_1 = \frac{K_6^R}{2\pi(K_6^R K_1^R - g_R{}^2)} \quad . \tag{6.9}$$

[The transition between phases C and C* is analogous to the transition between ferromagnetic and X-Y like phases in Sec. 4, for p = 6.] Some necessary conditions for stability of the C* phase are

$$\eta_\Delta > 4 \quad , \tag{6.10}$$

$$K_1^R > 2/\pi \quad , \tag{6.11}$$

$$K_6^R > 72/\pi \quad . \tag{6.12}$$

It should be noted that quasi-long-range order in tilt orientation always induces quasi-long-range order in the bond orientations; i.e., a phase with short range order in C_6 but quasi-long range order in C_1 is impossible. The right-hand portion of the C phase, labelled C_1 in Fig. 11, is a region where there would be no bond order if the molecules were not tilted. The correlation function $C_6(\vec{r})$ has algebraic decay at long distances only because of the coupling h between tilt and bond angles, and the amplitude of the correlations should be proportional to h^2. In the left hand portion of the C phase (labelled C_2), the bond angles would tend to order, (forming a hexatic phase) even in the absence of tilt. The amplitude of $C_6(\vec{r})$ will be independent of h in this region, and hence much larger than in the region C_1. Since there is no change in symmetry, there is no necessity for a sharp phase transition between the regions C_1 and C_2. However, there may be a first order transition in some cases.

B. Solid phases.

In addition to the fluid phases described above, there are two solid phases (B and H) indicated in Figure 11. These phases have true long-range order in the bond orientation,

$$\langle e^{6i\theta} \rangle = \text{const.} \times e^{6i\theta_0} \neq 0 \quad , \tag{6.13}$$

where θ_0 is the orientation of the crystal axis in the xy plane. The Frank constant K entering (6.2) should be considered infinite in the solid phases; however, we must now take into account coupling of the tilt orientation to the strain field of the crystal. Possible solid phases may then be understood in terms of the effective Hamiltonian

$$H/k_BT = \tfrac{1}{2}\int d^2r[2\mu u_{ij}{}^2 + \lambda u_{kk}{}^2 + 2w(u_{ij} - \tfrac{1}{2}\delta_{ij}u_{kk})s_is_j]$$

$$- h\int d^2r \cos[6(\phi(r)-\theta_0)] + \tfrac{1}{2}K_1 \quad d^2r(\vec{\nabla}\phi)^2 \qquad (6.14)$$

where the strain tensor $u_{ij}(\vec{r})$ is the symmetric derivative of the displacement field $\vec{u}(\vec{r})$ where u_{ij} is the strain tensor, μ and λ are the (bare) Lame elastic constants, and $\vec{s} = (n_x,n_y)$.

If the coupling proportional to w in (6.14) were neglected, one could apply the analysis of Sec. 4 to the tilt degrees of freedom. One would then find three solid phases: (i) an isotropic solid with short range order in the tilt orientation; (ii) an isotropic solid with quasi-long range tilt order; and (iii) an anisotropic solid with true longe range order in $\vec{s}$. We find, however, that the anharmonic coupling between phonons and $\vec{s}$ destabilizes the intermediate phase (ii) above. Presumably, this instability leads to a tilted anisotropic solid identical to (iii). One would then expect a line of phase transitions directly from an isotropic untilted solid (labelled B) to an anisotropic solid with tilt (labelled H), as shown in Fig. 11.

Phase boundaries shown as light solid lines in Fig. 11 are "Kosterlitz-Thouless" type phase transitons, with unobservable essential singularities in the specific heat, but with jumps in appropriate stiffness constants. The double lines represent transitions whose character has not been analyzed.

C. Relation to bulk smectic phases.

The labels A and C, in Fig. 11, were chosen because the corresponding phases have the properties of an isolated layer of the bulk phases known as smectic A and smectic C respectively.[63] Similarly, phases B and H correspond to the most commonly accepted description of the bulk smectic B and H phases, in which the smectic layers are believed to be two-dimensional solids. [A stack of two-dimensional solids with any finite coupling between the layers, will form (in thermal equilibrium) a three-dimensional solid, with conventional long-range translational order in all directions, as discussed below.] Recent X-ray measurements on the smectic B phase of the compound BBOA support this description.[60,82]

As pointed out by Birgeneau and Litster,[65] a stack of weakly coupled hexatic layers (the A* phase) might be expected to form a bulk liquid crystal phase, with short-range translational order parallel to the layers, but long-range order in the bond angle field, $<\psi> = 0$. It would certainly be very interesting if experimental evidence can be found for the existence of a bulk hexatic phase in some materials.

Hikami and Tsuneto[83] have studied in some detail the behavior of vortices in a stack of two-dimensional X-Y models, when there is weak coupling between the planes.[84] As they had also noted, similar considerations should apply to dislocations in a stack of smectic layers. We give here a crude argument.

Let us assume that there is a coupling between the translational order parameters in adjacent smectic layers, whose strength, per unit area, is denoted by γ. As a crude approximation, we may consider that in the hexatic phase, the translational order parameter $\rho_{\vec{G}}$ is coherent, in a given layer, over a region of area ξ^2, where ξ is the translational correlation length for an isolated layer. The effective coupling between coherent areas in adjacent layers would then be

$$\delta = \gamma\xi^2 < |\overline{\rho}_{\vec{G}}|^2 > \quad , \tag{6.15}$$

where $\overline{\rho}_{\vec{G}}$ is the spatial average of $\rho_{\vec{G}}$ over the region of size ξ^2, and the angular brackets represent a thermal average over phonon fluctuations. We find[15]

$$< |\overline{\rho}_G|^2 > \approx \xi^{-\eta_{\vec{G}}} \quad . \tag{6.16}$$

In order that there not be long range translational order, it is necessary that the coupling δ be small compared to T, or

$$\frac{\gamma}{T} < \xi^{\eta_G - 2} \quad . \tag{6.17}$$

A coupling energy of order (6.15) is also obtained if one considers the cost in energy if a dislocation pair of separation $\xi = n_{\text{free}}^{-\frac{1}{2}}$ appears in one layer but not in the adjacent layers.[83]

As the temperature is reduced in the hexatic phase, the correlation length will increase until (6.17) is violated. Presumably there will then be a first-order transition to a three dimensional solid (smectic B) phase.

We may note, finally that the unlocked tilted hexatic phase C* in Fig. 11 should not have any analogue in bulk smectics. Coupling between layers would be expected to convert quasi-long-range order to true long range order for the tilt orientation parameter $\vec{s}$. The coupling term $h \cos 6(\theta-\phi)$ will then lock the phase of $\langle\vec{s}\rangle$ to the phase of the bond orientation parameter $\langle\psi\rangle$.

BIBLIOGRAPHIC NOTE

There have been several recent conferences and summer institutes where phase transitions in two dimensional systems were discussed, including the NATO Advanced Study Institute on "Ordering in Strongly-Fluctuating Condensed Matter Systems," Geilo, Norway, April 1979, and the Ettore Majorana Summer School on "Phase Transitions in Surface Films," in Erice, Sicily, June 1979. The proceedings of these conferences, when published, should provide useful reviews of experimental and theoretical developments in the field. Other recent reviews have been written by Kosterlitz and Thouless[6], Barber[85] and Erzan[86].

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