Chapter 1

Early Work on Defect Driven Phase Transitions

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This article summarizes the early history of the theory of phase transitions driven by topological defects, such as vortices in superfluid helium films or dislocations and disclinations in two-dimensional solids. We start with a review of our two earliest papers, pointing out their errors and omissions as well as their insights. We then describe the work, partly done by Kosterlitz but mostly done by other people, which corrected these oversights, and applied these ideas to experimental systems, and to numerical and experimental simulations.

1.1. Introduction

The idea that certain phase transitions might be driven by the occurrence of an equilibrium concentration of defects such as dislocations in solids or quantized vortices in superfluids is almost as old as the recognition that such defects have an important role in the mechanical or electrical properties of such materials. Indeed, in Onsager’s incredibly brief initial note on the existence of quantized vortices in superfluid helium, the possibility of a vortex-driven transition from the superfluid phase to the normal fluid phase is mentioned,¹ and this possibility was later presented by Feynman² in a much more accessible form. There are also discussions of the idea that the spontaneous formation of an equilibrium density of dislocations in solids could lead to the transition from a rigid solid to a liquid with viscous flow. Such models involve handling the statistical mechanics of line defects...
in a three-dimensional medium, and such problems are notoriously difficult to handle.

1.2. One-Dimensional Ising Model

The first exposure of one of us (DJT) to the ideas that were to prove important in the theory of defect driven phase transitions happened as a result of a visit to Bell Labs. There I was told by Philip Anderson of the work with his student Gideon Yuval and his colleague Don Hamann on the solution of the Kondo problem (for a magnetic impurity in a low temperature metal), by means of a transformation of the problem to a one-dimensional Ising model with a long-range interaction between the spins falling off with distance like $1/r^2$. They recognized that such an inverse square law for the interactions had a slower fall-off with distance than those known to give no equilibrium magnetization, and faster than those known to have magnetization at sufficiently low temperatures. Anderson asked me if I knew anything about this intermediate case, so I thought about it, and, on the train back to Stony Brook, realized that the argument on the last page of the 1958 translation of Landau and Lifshitz, *Statistical Physics*, could be adapted to give a plausible answer to this problem, so I tried it out on some of the statistical mechanics faculty and visitors at SUNY Stony Brook, such as Bob Griffiths and Barry McCoy.

The basic idea of the Landau and Lifshitz argument is to consider the statistical mechanics of the domain walls between blocks of spin up and spin down. If $a$ is the spacing between spins, then $a$ is also the length occupied by each domain wall. The entropy is the same as the entropy in a one-component, one-dimensional hard “sphere” gas, so that, in a system of length $L$ with $p$ domain walls, the entropy is

$$S \approx k_B p \ln(L/pa),$$

and so it is logarithmically divergent in the limit of large $L$, fixed $p \neq 0$. In the case of a finite range interaction the energy per domain wall is finite in the limit of large $L$, so that at any nonzero temperature the entropy dominates, there is a nonzero concentration of domain walls, and zero equilibrium magnetization, in this limit.

In the particular case of a $Ja^2/r^2$ interaction between spins, the energy of a single domain wall at $x$ can be approximated as

$$E = 2J \int_{-L/2}^{x-a/2} \int_{x+a/2}^{L/2} \frac{1}{(x_2 - x_1)^2} dx_2 dx_1 = 2J \ln \left(\frac{(L + a)^2}{4 - x^2}\right) \approx 2J \ln \frac{L}{4a},$$

(1.2)
for \( x \) in the interior, well away from the boundaries at \( x = \pm L/2 \). At low temperatures the free energy \( F = E - TS \) is dominated for large \( L \) by the energy, so there are no free dislocations in equilibrium, but for \( T > J/k_B \) the entropy dominates, free domain walls are thermodynamically stable, and there is no net magnetization.

The argument that was published in 1969\textsuperscript{10} had a few more refinements. In particular, although isolated domain walls are forbidden at low temperatures in the thermodynamic limit, pairs of domain walls, which provide a nonzero magnetization density, are not forbidden. A pair of domain walls a distance \( na \) apart contains \( n \) spins in the reverse direction, and has energy

\[
E_n \approx 4Ja^2 \ln n.
\]

(1.3)

A concentration \( c_n \) of such pairs of domain walls reduces the magnetization \( M \) by

\[
-\delta M = \sum n^2 nc_n,
\]

(1.4)

and this reduces the magnetization from its zero-temperature value of unity as the temperature is increased. This has the effect of reducing the coefficient of the \( \ln L \) term in Eq. (1.2) for the domain wall energy by a factor approximately equal to \( \delta M(T) \), and so the inequality that determines the possibility of isolated domain walls, or of the dissociation of domain wall pairs into free domain walls, becomes

\[
k_B T \geq JM.
\]

(1.5)

I was startled by the conclusion that the magnetization would decrease monotonically as the temperature was raised, but that, rather than decreasing continuously to zero, must jump to zero when the inequality (1.5) is satisfied. This is not a first order transition, since the energy is a continuous function of \( T \).

This result was confirmed in more careful theoretical work by Dyson,\textsuperscript{11} Fröhlich and Spencer\textsuperscript{12} and by Aizenman \textit{et al.}\textsuperscript{13} Initially, apart from its association with the scaling theory of the Kondo effect,\textsuperscript{6} it did not seem much more than a curiosity, but its wider significance was soon appreciated.

1.3. Vortex Driven Transitions in Superfluid Films

In 1971 two things came together for us. Thouless decided to give a graduate course on superfluidity and superconductivity, and, in explaining that the energy of a quantized vortex in a thin film of superfluid depends logarithmically on the area of the film, realized that the same entropy–energy balance
that occurs in the $1/r^2$ Ising model should also occur in the natural vortex model for a neutral superfluid film. At about the same time, Kosterlitz left Torino and arrived in Birmingham in his second post-doctoral position; he began looking for an area of physics outside elementary particle theory to try out. He was enticed into condensed matter physics by our colleague Eric Canel, and the two of us started talking about vortex-driven transitions in superfluid films. This was the start of our collaboration to explore the possibility of a new sort of phase transition in two-dimensional systems.

The flow velocity in a superfluid condensate is $\hbar/M_A$ times the gradient of the phase of the condensate wave function, where $M_A$ is the atomic mass (or pair mass in the case of fermion superfluidity), and so the flow velocity is always the gradient of a potential function. The appearance of uniform rotation in superfluid helium was a paradox resolved by Onsager’s suggestion that it was the effect of an approximately uniform distribution of quantized vortex lines in the rotating liquid, with the microscopic velocity being a sum of terms $\hbar \nabla \phi_i / M_A$, where $\phi_i$ is the azimuthal angle referred to the core of a particular vortex $i$. This general picture was confirmed by the experimental work of Hall and Vinen in 1956.

In three dimensions the energy and entropy of interacting vortex lines are complicated to calculate, and the needed approximations are unconvincing. In a two-dimensional system, such as a thin film of superfluid helium, the vortices are quantized, with circulation an integer multiple of $\hbar/M_A$. The only degrees of freedom of a quantized vortex are the two coordinates of the position of the vortex core, which, in a classical theory of vortex dynamics, such as the one formulated by Kirchhoff, are conjugate dynamical variables, and which should therefore be governed by an uncertainty relation in a quantized theory. This uncertainty relation quantizes the area $A = \pi R^2$ into cells of area $\pi a_1^2 = M_A/\rho_s$, and this gives the entropy per vortex as

$$S_v \approx k_B \ln(L^2/a_1^2). \quad (1.6)$$

The vortices can have positive or negative circulation $\pm \hbar/M_A$. The energy of an isolated vortex near the center of a disk of superfluid of radius $R$ can be written as

$$E_V \approx 2\pi \int_{a_0}^{R} \rho_s \left( \frac{\hbar}{M_A r} \right)^2 r dr = 2\pi \rho_s (\hbar/M_A)^2 \ln(R/a_0). \quad (1.7)$$

Here $a_0$ is the vortex core radius, the healing distance over which the superfluid density is suppressed by the high speed near the core, and $\rho_s$ is the superfluid density per unit area, which is defined and measured in terms of the energy density for a given superfluid flow velocity. If the isolated vortex
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is not close to the center of the system, but is close to one of the boundaries, the energy is reduced by the backflow produced by the boundary, just as the energy of a free electrostatic charge is reduced by the charge density induced in a neighboring conducting surface, so that at distance \( l \) from the boundary it becomes

\[
E_V(l) \approx 2\pi \int_{a_0}^{l} \rho_s \left( \frac{\hbar}{MAr} \right)^2 r dr = 2\pi \rho_s \left( \frac{\hbar}{MA} \right)^2 \ln(l/a_0). \tag{1.8}
\]

There is obviously a close analogy between Eqs. (1.1) and (1.2) for the one-dimensional Ising model with \( 1/r^2 \) interactions, and Eqs. (1.6)–(1.8) for vortices in a superfluid thin film. In analogy with Eq. (1.3) for the Ising model, the energy of a pair of oppositely rotating vortices with circulation \( \pm h/MA \) separated by a distance \( d \) is given as

\[
E_{vp}(d) = 2\pi \rho_s \left( \frac{\hbar}{MA} \right)^2 \ln \frac{d}{a_0}. \tag{1.9}
\]

Comparison of Eqs. (1.6) and (1.7) shows that the condition for stability of the superfluid against the appearance of isolated vortices is

\[
k_B T \leq \pi \rho_s (h/MA)^2. \tag{1.10}
\]

These arguments were given in our 1972 and 1973 papers.\textsuperscript{16,17} However we got an incorrect factor of \( MA/M^* \), where \( M^* \) is an effective mass, in our derivation. A proper derivation was given by Nelson and Kosterlitz.\textsuperscript{18} The corrected result is important, because the parameter-free relation between the critical temperature and superfluid density can be, and was, experimentally verified. A straightforward explanation for this robust relation between the maximum temperature for stable superfluidity comes from the fact that the coefficient of the logarithm in the expression (1.7) depends on the average flow induced on a circuit at large distance from the vortex core by the \( 2\pi \) twist of the phase angle, and the superfluid density is also defined by the energy induced by a twist of the phase angle imposed over a large area. Therefore, even if nonuniformity of the substrate causes nonuniformity of the superfluid film, it is the same average that comes into the expression for superfluid density and for vortex energy.

For a short while we could congratulate ourselves on discovering completely new physics. It did not last long, because, on a trip to Paris, Thouless met Paul Martin, who was spending a sabbatical there, and he said that he had heard the story before, from some Russian visitor who knew of Berezinskii’s work. This was too early for us to have the translations available, we had little knowledge of Russian between us, and we cannot
remember why we did not get a colleague to translate the papers for us. We cited two papers by Berezinskii;\textsuperscript{19,20} the first of these is irrelevant, but the second anticipated our published work by a year. For reasons we do not know, and about which it is inappropriate for us to speculate, our work had more impact than Berezinskii’s, and was much more often quoted. There seem to have been nearly 2200 papers published since 1972 that mention our work in the title or abstract, only 3 of which were published in the first five years. Of these articles, 1700 are classed as purely theoretical and 500 as experimental, according to Inspec.

We have our own stories of missed opportunities. One of us (DJT) went down to the University of Sussex to give a seminar to Douglas Brewer’s group there. I knew that he and his collaborators had done good work on superfluid films, and hoped that he would follow up our result that the superfluid density should have a discontinuity at the superfluid–normal critical temperature. Douglas was politely interested, and told me that Isadore Rudnick’s group at UCLA had done some experiments on superfluid films, and had found such a discontinuity,\textsuperscript{21,22} but that a careful reanalysis of their data had made this unexpected discontinuity disappear. I failed to look up the UCLA paper, and Douglas did not follow up on our ideas. There are two morals in this story. One is that theorists should read the relevant experimental literature carefully, and the other is that experimentalists should not stop checking their results just because they are consistent with existing theory.

1.4. Other Systems with Defect-Mediated Transitions

At that time the main subject of interest for theorists in statistical mechanics was the “universal” nature of critical behavior, pioneered by Cyril Domb, Michael Fisher,\textsuperscript{23} Leo Kadanoff and many others, which led to the renormalization procedure to determine critical exponents, described in the papers of Kenneth Wilson\textsuperscript{24} and Wilson and Fisher.\textsuperscript{25} The argument was that, as the critical point is approached in a transition such as the liquid–vapor transition, length scales get larger and larger, and the details of the mechanism become irrelevant. Close to a critical point only broad features, such as the dimensionality of the order parameter, are important. It was therefore natural to extend the arguments to other two-dimensional systems which have similar defects with a similar long-range interaction between them. In some cases we did this successfully, in other cases we got important details wrong, and many other cases we did not think about.

In the mid 1930s Peierls had produced general arguments\textsuperscript{26,27} that showed
that in two-dimensional systems with an order parameter with more than
one degree of freedom, such as a superfluid, or a magnet with magnetism
isotropic in two- or three-dimensional space, long-wavelength fluctuations of
the azimuthal angle of the magnetization would result in the average mag-
etization tending to a zero limit as the system got large. Twenty years
later this result was derived more carefully by Mermin and Wagner\textsuperscript{28} and by
Hohenberg.\textsuperscript{29} Although, later authors had proved that the average magneti-
zation must be zero, a number of people pointed out that it was not proved
whether higher order correlations of the spins could have a nonzero limit
at low temperatures, but a vanishing limit at higher temperatures. This
would still allow for a critical point at the temperature where this transition
occurred.

In this section we describe the theory roughly as we saw it in the early
1970s, and point out what we missed and where we went astray. In Sec. 1.6
we describe the essential modifications of the work described in this section
that were made in the late 1970s.

1.4.1. \textit{Two-dimensional magnetic systems}

Magnetic systems are usually regarded by theorists as the standard for clas-sifying the universality classes of other systems of transitions with critical
points or lines. They are not always readily available experimentally, since
most real magnetic systems are solids, and the lower symmetry of a solid as
compared with an isotropic liquid, either because of the intrinsic symmetry
of an ideal crystal, or because of the local effects of impurities, may compli-
cate the analysis of results. Furthermore, ferromagnetic systems are more
complicated than antiferromagnetic systems, since the long-range interaction
between the aligned magnetic dipoles gives rise to the formation of domain
walls. The basic example of the Ising model universality class has a nearest
neighbor interaction between the $z$ components of the spins on a regular
lattice, in two, or three dimensions, but a weaker interaction between the
other two components of spin does not change the behavior near the critical
temperature and close to zero magnetic field. There is good evidence that
the order–disorder transition in a binary alloy and the gas–liquid transition
in a one-component fluid are also in this universality class.\textsuperscript{30} In the classical
Heisenberg model the spin can point in any direction in space, and the inter-
action energy of any neighboring pair of spins is proportional to the scalar
product of the two neighboring spins. In the planar spin model there is an
interaction between neighboring spins which is stronger for the $x, y$ com-
ponents than it is for the $z$ components, and is unchanged by rotations of the
spins about the $z$ axis. It is this planar spin model in a two-dimensional system which is thought to be in the same universality class as the superfluid film; the real and imaginary parts of the local value of the condensate wave function correspond to the $x$ and $y$ components of the spin. The spin system is two-dimensional if it is thin enough that spin directions on opposite faces of the film are strongly correlated. The analog of a vortex is a point in the two-dimensional space around which the projection of the spin direction in the plane rotates by $\pm 2\pi$, and we often use the term ‘vortex’ to describe such a structure in a spin system.

At large distances from the vortex core the energy per nearest neighbor bond is proportional to

$$|J_x|(1 - \cos \delta \phi) \approx \frac{|J_x|}{2} (\delta \phi)^2,$$

(1.11)

where $J_x = J_y$ is the strength of the in-plane coupling, and $\delta \phi$ is the difference between the azimuthal angles of the two spins. Summation of this over the bonds surrounding a vortex will give close approximations to the integrals shown in Eqs. (1.7) and (1.8). In Sec. 1.2 the result of such a modification in the domain wall energy led to an increase in the magnetic susceptibility with rising temperature, while in Sec. 1.3 the decrease in the vortex energy leads to a decrease in the superfluid density as the temperature rises, as is discussed in more detail in Sec. 1.5. For the planar magnetic system the quantity that corresponds to the magnetization in the one-dimensional inverse square law magnet and to the superfluid density in the two-dimensional superfluid is the spin-wave stiffness, which is a measure of the energy associated with a progressive in-plane twisting of the magnetization direction. This is analogous to the superfluid density, because the superfluid density measures the extra energy density associated with a steady supercurrent, and the superfluid velocity, by definition, is given by $\hbar/m_B$ times the gradient of the phase of the condensate, where $m_B$ is the boson mass.

### 1.4.2. Isotropic Heisenberg model

Although analysis of the high temperature series by Stanley and Kaplan\textsuperscript{31} seemed to show a critical temperature both for the planar spin model and for the Heisenberg model in two dimensions, slightly later work by Stanley\textsuperscript{32} and by Moore\textsuperscript{33} showed that the indication of a phase transition was much clearer for planar spins than for the isotropic Heisenberg model. This is consistent with the argument that we gave, that, for the Heisenberg model, there should only be a finite energy barrier separating topologically different
states. A more careful argument of this sort was given by Belyavin and Polyakov.\textsuperscript{34}

The argument is that for the planar spin model and its analogs there is a topological invariant characterizing a vortex-like configuration, which is the winding number of the polar angle $\phi_s$ of the planar spin direction,

$$n_w = \frac{1}{2\pi} \int d\phi_s. \quad (1.12)$$

Since $\phi_s$ is single valued modulo $2\pi$, $n_w$ must be integer. Furthermore, for many of the systems we discuss, at low temperatures there is an energy barrier between configurations with different winding numbers whose magnitude diverges logarithmically with the linear dimensions of the system, so that spontaneous fluctuations of the winding numbers are suppressed. The simplest way of adding a free ‘vortex’ is to add it close to the boundary of the two-dimensional space in which the system resides, in which case, as Eq. (1.8) shows, the energy is small. When this new vortex is pulled away from the surface, its energy increases logarithmically with the distance from the surface. Alternatively, two vortices of opposite sign can be created close to one another, and then pulled away from one another, so the energy increases logarithmically as their separation increases.

For the isotropic Heisenberg model there is no loop integral defining a topological invariant, since any loop on the 2-sphere that defines the directions of the spins, characterized by the polar angles of the spin directions, can be shrunk continuously to a point. If the spin direction on the distant boundary of the two-dimensional space tends to $\theta = 0$ then there is an invariant integral over all space

$$n_S = \left(\frac{1}{2\pi}\right) \int dx \int dy \left[ \partial \frac{\partial \cos \theta \partial \phi}{\partial x} - \partial \frac{\partial \cos \theta \partial \phi}{\partial y} \right] = \frac{\Delta \phi}{2\pi}, \quad (1.13)$$

where $\Delta \phi/2\pi$ is the winding number of $\phi$ at the distant boundary at which $\theta = \pi/2$. This measures the number of times the mapping of the $xy$ space onto the sphere defined by the polar angles covers the $\theta\phi$ sphere. This topological invariant was known to Gauss. The excitation away from the $\theta = 0$ fully aligned ground state, to a state in which $n_S = 1$, is known as a skyrmion, in honor of our former colleague and boss, who introduced this as a model for an elementary particle.\textsuperscript{35} For an interaction that can be approximated as proportional to $|\nabla S|^2$ this excitation has a finite, scale-independent, energy, so that skyrmions can be excited with nonzero density at arbitrarily low temperatures, and there is no phase transition to a magnetized state at a nonzero temperature.
Theoretical arguments were advanced for the importance of skyrmions, rather than spin waves, as excitations giving the response of certain quantum Hall materials to magnetic fields.36,37 Experimental evidence in support of this has accumulated,38 and there is a recent review by Ezawa and Tsitsishvili.39

1.4.3. Two-dimensional Coulomb plasma

The discussion of the interaction of vortices and of the importance of the logarithmic dependence of the energy of a vortex pair on the distance between the two, which was discussed in Sec. 1.3, suggested that a useful model for the statistical mechanics of these vortices would be a two-dimensional plasma of positive and negative charges. The interaction energy between the charges $q_1, q_2$ has to be proportional to $q_1 q_2 \ln |\mathbf{r}_1 - \mathbf{r}_2|$, and this is not what happens for real electric charges confined to a thin layer. We therefore do not know of a real system of charges that behave like this, but we can use some of the insights gained from work on three-dimensional systems, such as ionic solutions.40

For a dilute plasma, such as occurs in the upper atmosphere, the ions may be bound together in pairs as neutral diatomic molecules, whose diameter depends on the sizes of the two ions, or the ions may be separated from their opposite partners. In response to an electric field, either external, or from one of the free ions, the surrounding plasma is polarized, and this has the effect of screening out the long-range effect of the field due to an ion. In analogy with the dynamics of vortices, for which the $x$ and $y$ coordinates are conjugate variables (a result which Horace Lamb15 quotes from a textbook on Mechanics by Kirchhoff), the kinetic energy is constant, and quantized in units of two-dimensional area. In the case of a logarithmic dependence of the energy on separation, this screening is incomplete, and we had to adapt renormalization group methods developed by Anderson, Yuval and Hamann4,6 and by Wilson and Fisher24,25 to solve this problem. Our initial efforts to make these methods fit our problem were inadequate,17,41 and later developments are discussed in more detail in Sec. 1.5.

1.4.4. Two-dimensional crystals

In our early papers16,17 we discussed the analogy between the vortex-driven superfluid to normal transition in helium films and an analogous melting transition between solid and liquid phases in thin films. We got part of this right, but missed some essential features. These missing features were pointed out and corrected by Halperin and Nelson42 and by Peter Young.43
There are two important differences between liquids and solids. The most obvious one is that an ideal solid is rigid and does not yield to a small stress, but recovers its original shape when the small stress is removed, while a liquid will flow without any memory of its original shape. The second difference is that a liquid is isotropic, with no preferred directions in space, while most solids are crystalline, even if their crystal structure is not immediately obvious to the eye, and a single crystal of a solid has different mechanical, electrical and optical properties in different directions. This crystal structure was first studied in detail by X-ray crystallography, which was developed a hundred years ago by Laue and his collaborators and by the Braggs. In fact, the possible periodic arrays that could be formed by identical atoms were identified, and classified by the use of group theory, and by the examination of the symmetries of real crystals, during the last half of the nineteenth century.

Despite these sharp differences between typical solids and typical liquids, there are actually various intermediate examples known. For example, ordinary silica-based glass has no orientational order, but glasses have existed for hundreds or even thousands of years without showing any signs of losing their shape because of flow induced by gravitational forces. In contrast there are materials, now known as liquid crystals, which flow freely like liquids, but which have local orientational order. Since the 1930s it has been known that it is the presence of dislocations in imperfect metals that allows them to flow, or creep, under a shearing stress, although this is not like the flow of a liquid, whose rate is proportional to the applied stress, but the rate of creep is very slow under a low stress. This led to the idea that the melting transition in a solid might be due to the spontaneous appearance of thermodynamically stable dislocations at the melting temperature.  

In a regular triangular lattice, even if it is disordered by thermally excited sound waves, each atom has six immediate neighbors. Even when thermal excitation of vacancies and interstitials is taken into account, the shape remains stable against stress, and the anisotropy revealed by the X-ray diffraction pattern remains. In 1934 papers appeared more or less simultaneously, written by E. Orowan, M. Polanyi, and G. I. Taylor, which described how what are now known as dislocations can greatly reduce the energy barriers to the flow of a solid in response to stress. In the ideal two-dimensional case, shearing stress can only be relieved by a whole line of atoms slipping over an adjacent line, and this involves an energy barrier proportional to the length of the line. If there are dislocations in the solid, which involve partial extra (or missing) lines of atoms that terminate at the
Fig. 1.1. A dislocation in a triangular lattice with an extra line of particles inserted. The dashed line is a Burgers circuit which would close in a perfect lattice but fails to close by a Burger’s vector $\mathbf{b}$. Note that the dislocation core has a five- and a seven-fold coordinated particles one lattice spacing apart and the Burger’s vector, $\mathbf{b}$, is perpendicular to the bond joining these. These particles can be regarded as two disclinations separated by one lattice spacing. Reprinted from Fig. 27 of Ref. 50, with permission from Elsevier.

dislocation core inside the solid, as shown in Fig. 1.1, the dislocation can respond to shear stress, with the help of thermally activated vacancy sites and interstitials, by changing its track one or two atoms at a time, so the energy barrier is much lower. The presence of such dislocations in most solids, particularly in metals, explains why plastic flow does actually occur in them, particularly at high temperatures; certain metals, such as copper, lead and gold are quite soft when their purity is high, because their dislocations are free to move.

For each dislocation in a plane lattice there is an extra row of atoms which starts at the site of the dislocation and terminates at the boundary of the crystal. As a result, a path from atom to atom which would be a polygon around the site of the dislocation fails to meet by an amount known as the Burgers vector of the dislocation, as is shown in Fig. 1.1. This vector is perpendicular to the extra row of atoms. There can be bound pairs of dislocations with opposite Burgers vectors, which correspond to extra (or missing) finite rows of atoms between the positions of the two opposite dislocations.

We argued that, since the dislocation in two dimensions is a point defect, like the vortex in a superfluid, and the energy of an isolated dislocation depends logarithmically on the size of the system, there should also be a defect driven melting transition in a two-dimensional solid at the temperature
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Fig. 1.2. $\pm \pi/3$ disclinations in an underlying triangular lattice. On a circuit enclosing the disclination cores, there is an orientational mismatch by $\pm \pi/3$: $\oint_C d\theta = 2\pi \pm \pi/3 = 2\pi \pm \pi/3$. Reprinted from Fig. 28 of Ref. 50, with permission from Elsevier.

where the energy and entropy terms balance one another.\textsuperscript{16,17} There were two significant errors in this argument, which Halperin and Nelson,\textsuperscript{42} and Young\textsuperscript{43} pointed out. The first error is that the coefficient of the interaction energy of a dislocation pair is not isotropic, like the interaction between vortices, but depends on the angle between the displacement of one dislocation from the other and the direction of the Burgers vector (the normal to the line of extra atoms). The more important correction is that the presence of free dislocations is not enough to destroy the orientational order of the solid, but a further transition must occur.

The point defects that destroy orientational order are known as disclinations,\textsuperscript{44} which in a two-dimensional triangular lattice are groups of nearest neighbors that form a pentagon or heptagon rather than the hexagon of the typical group of neighbors. In Fig. 1.1 one can see that the core of the dislocation is made up of one pentagon and one adjacent heptagon, which can be regarded as a pair of oppositely charged disclinations in nearest neighbor positions.\textsuperscript{44} Isolated disclinations are shown in Fig. 1.2. Along a loop that winds once round such a disclination, parallel transport of a coordinate frame oriented with the local crystal axes would rotate it by an angle $-2\pi/5$ or $+2\pi/7$, and $\pm \pi/3$ relative to an undistorted, triangular reference lattice, according to the sign of the disclination. A random set of positive and negative dislocations does not destroy orientational order in a solid, and so the transition from ordered, rigid solid to disordered fluid can take place through two distinct defect-driven phase transitions.\textsuperscript{42,43} At the first transition, the dislocation pairs that form at low temperatures become dissociated to form
an oriented fluid known as a *hexatic liquid crystal*. Disclinations play no role in the melting of an elastic solid because there is true long range orientational order and the energy of an isolated disclination is proportional to the area of the elastic system. At the higher temperature transition, the disclination pairs that form a free dislocation dissociate to create an unoriented fluid of the usual type. This is discussed in more detail in Secs. 1.6.3 and 1.7.2.

Shortly after we had written this up and distributed preprints we received a preprint from Feynman which contained the same argument, but with a different expression for the dependence of the energy of a free dislocation on the elastic moduli. Feynman’s disagreement with us was worrying, but we found to our relief that we had got it right. Feynman did not actually publish his preprint, but an account of it was included in a paper by Elgin and Goodstein.

1.4.5. *Thin film superconductors*

A sufficiently thin film of superconductor can be regarded as two-dimensional and can be described by Ginsburg-Landau free energy for a charged condensate of Cooper pairs,

\[
F[\Psi] = \int d^2r dz \left\{ \frac{1}{2m^*} \left( -i\hbar \nabla - \frac{e^*}{e} A \right) \Psi \right\}^2 \\
+ \frac{1}{2} r(T)|\Psi|^2 + \frac{1}{4} u|\Psi|^4 + \frac{B^2}{8\pi} - \frac{\mathbf{H} \cdot \mathbf{B}}{4\pi} \right\}. \tag{1.14}
\]

The field \( \Psi(\mathbf{r}) \) is a coarse grained Cooper pair condensate wave function which is finite in the plane of the film, \( \mathbf{A}(\mathbf{r}, z) \) is the magnetic vector potential, \( \mathbf{B}(\mathbf{r}, z) = \nabla \times \mathbf{A}(\mathbf{r}, z) \). The parameter \( r(T) \) is negative below the critical temperature of the film in the absence of a magnetic field, and \( u \) is positive and assumed to be temperature independent. Here, \( \mathbf{r} = (x, y) \) is a point in the film which lies in the plane \( z = 0 \), the effective mass \( m^* = 2m_e \), and \( e^* = 2e \). The important difference between the uncharged superfluid of \(^4\text{He}\) and a charged superfluid of a superconductor is that a vortex in a superconductor has a circulating electric current producing an associated magnetic field, \( \mathbf{B}(\mathbf{r}, z) \), which exists in the space outside the film at \((\mathbf{r}, 0)\). The behavior of a superconducting film was first discussed by Pearl who found that the circulating current of a vortex at \( \mathbf{r} = 0 \) falls off as \( 1/r^2 \), instead of exponentially as in a bulk superconductor. Also, the screening length in a 2D superconducting film is \( \lambda_{2d} = \lambda_0^2/d \), where the London penetration depth \( \lambda_0 \) is of order 1 \( \mu \text{m} \), and \( d \) is the film thickness. To ensure
that a real film can be approximated by a 2D film, one must have $d \ll \lambda_0$ so that there is no variation over the film thickness.

On scales larger than the superconducting coherence length, $\xi_0 = \sqrt{\hbar^2/(m^*|r(T)|)}$, which is the length over which the order parameter grows from zero at a vortex core to its mean value, $|\Psi_0| = \sqrt{-r(T)/u}$, well away from the core, the phase only approximation $\Psi(r, z) = \Psi_0 e^{i\theta(r)}$ is valid, and the free energy of Eq. (1.14) becomes

$$F = \int d^2r dz \left\{ \frac{\rho_0}{2} \left( \frac{\hbar}{m^*} \right)^2 \left( \nabla \theta - \frac{e^*}{\hbar c} A \right)^2 + \frac{1}{8\pi} (\nabla \times A)^2 \right\} + \text{constant},$$

(1.15)

where $\rho_0 = m^*|\Psi_0|^2$ is the mass density of the Cooper pairs. From the variational equation $\delta F/\delta A = 0$, one obtains

$$\nabla \times (\nabla \times A) = \nabla \times B = \frac{4\pi e}{c} = 4\pi |\Psi_0|^2 \frac{e^* \hbar}{m^* c} \left( \nabla \theta - \frac{e^*}{\hbar c} A \right),$$

$$\Rightarrow J(r, z) = e^*|\Psi_0|^2 \frac{\hbar}{m^*} \left( \nabla \theta - \frac{e^*}{\hbar c} A \right).$$

(1.16)

To see the effect of the magnetic field $B$ due to a set of vortices in the superconducting plane at $z = 0$, we follow the analysis of Nelson’s book by assuming that the superconducting current is in the plane $z = 0$, so that

$$-\nabla^2 A(r, z) + \frac{1}{\lambda_{\text{eff}}} A_{2d}(r) \delta(z) = \frac{m\phi_0}{2\pi\lambda_{\text{eff}}} \hat{z} \times \frac{r}{r^2} \delta(z),$$

(1.18)

since $\theta(r)$ due to the vortex at the origin $r = 0$ is $\nabla \theta(r) = 2\pi m(\hat{z} \times r)/r^2$, and $A_{2d}(r) = A(r, z = 0)$. This can be solved by taking Fourier transforms, with the result that the current in the superconducting plane behaves like a neutral superfluid for $r \ll \lambda_{\text{eff}}$ with

$$J_{2d}(r) = \frac{mc\phi_0}{8\pi^2 d\lambda_{\text{eff}}r} \hat{\theta},$$

(1.19)

and, for $r \gg \lambda_{\text{eff}},$

$$J_{2d}(r) = \frac{mc\phi_0}{4\pi^2 d r^2} \hat{\theta}.$$
This translates into a $\ln r$ vortex–vortex interaction as in a neutral superfluid for $r < \lambda_{\text{eff}}$, and a $1/r$ interaction for $r > \lambda_{\text{eff}}$.

Since the interaction between vortices in a superconducting film falls off faster than $\ln r$, this implies that there is no transition to a true superconducting state in the thermodynamic limit. However, since the effective penetration depth $\lambda_{\text{eff}}$ can be as large as $O(10^{-2})$m, which is larger than the typical film, the behavior of the system at low temperatures will be indistinguishable from that of a true phase transition rounded by finite size effects. The most common measurement on a superconducting film is the IV characteristics at various temperatures $T$. The theory discussed here is not adequate to predict the IV characteristics because the voltage $V$ produced by the applied current $I$ is due to the unbinding of vortices, whose subsequent motion produces the measured voltage $V$.\(^{55}\)

1.5. Scaling Theory

Kosterlitz and Thouless did have one advantage over other more knowledgeable workers who were investigating these low dimensional systems in which fluctuations dominate the behavior. Thouless had always been a bit of a maverick who loved unusual physics problems and Kosterlitz was too ignorant of statistical mechanics to realize that the problem of phase transitions in 2D magnets, superfluids and crystals was either absurd or too difficult to attempt. It might be absurd because of some well known rigorous theorems about the absence of long range order at any finite temperature in such systems.\(^{28,29,56}\) Almost all physicists took these theorems to mean that a phase transition could not exist in these systems, implying that the problem was absurd. However, careful reading of Mermin’s papers revealed that he did not exclude the possibility of a transition between different states at a finite temperature, but he did prove the absence of true long range order at any $T > 0$. The conventional wisdom at that time was based on Lev Landau’s mean field theory,\(^{57}\) in which a transition between low and high $T$ states involves the destruction of long range order, which was assumed to characterize the low $T$ state, and to be absent in the high $T$ state. Hence, the absence of long range order for all finite temperatures meant that the idea of a phase transition was unlikely, although Imry and Gunther had pointed out that the formation of a two-dimensionally ordered phase would lead to a characteristic signal in the X-ray scattering. Even if a transition did exist, it was clear that large, strongly interacting fluctuations were involved. There was a major dearth of techniques to handle such strongly interacting degrees of freedom, with the exception of perturbation expansions which were tech-
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nically difficult and whose meaning was obscure, so the chances of success were vanishingly small.

Undeterred by the general view that the problem was either absurd or impossible, Kosterlitz, out of ignorance, and Thouless, out of curiosity, went ahead and essentially solved the problem. In their first paper on superfluids and solids in two dimensions, the concept of topological order was introduced for systems which have no conventional long range order at any finite temperature. There it was argued that the important quantity which distinguishes an ordered phase from a disordered one is the rigidity of the system, and this is controlled by the presence or absence of free dislocations or vortices. In the ordered phase, these topological excitations are bound in pairs, but, when they unbind and become free to move, the rigidity vanishes and the two-dimensional solid responds to a shear stress like a fluid. Exactly analogous arguments can be constructed in terms of the unbinding of vortex pairs into free vortices to discuss the destruction of superfluidity in a two-dimensional film of superfluid $^4$He. The argument is as follows: the energy of an isolated vortex in a $2D$ $XY$ magnet of size $L$ with nearest neighbor coupling constant $J$ is $2\pi J \ln(L/a)$ and the associated entropy is $k_B \ln(L^2/a^2)$ so that the free energy is just $\Delta F = (\Delta E - T \Delta S) = 2(\pi J - k_B T) \ln(L/a)$. For a very large system $L \to \infty$, $\Delta F \to +\infty$ for $k_B T < \pi J$, which corresponds to no free vortices and finite rigidity, while, for $k_B T > \pi J$, $\Delta F \to -\infty$, the probability of thermally activated vortices approaches unity. This means that the generalized rigidity vanishes or that the system is disordered.

Once the mechanism and the relevant excitations had been identified, Kosterlitz and Thouless decided to attempt to make their ideas more quantitative. This took them into completely unexplored regions of statistical mechanics. The first essential step was to write the Hamiltonians for the superfluid film and the $2D$ solid in terms of the relevant excitations. We knew that the lowest energy excitations, spin waves in the magnet and phonons in the solid, although they destroyed the conventional long range order in two-dimensional $XY$ magnets, superfluids and solids, these excitations did not induce true disorder with the characteristic exponential decay of correlation functions in a high temperature phase, nor did they reduce the rigidity of the systems. Define the phase angle $\theta(r)$ of the order parameter $\psi(r)$ by

$$
\psi(r) = |\psi| e^{i\theta(r)}, \quad \theta(r) = \phi(r) + \sum_R n(R) \Theta(r, R), \quad (1.21)
$$

where $\phi(r)$ corresponds to the smooth variations of the phase angle $\theta(r)$, and $\Theta(r, R) = \tan^{-1}(y - Y)/(x - X)$ is the contribution to $\theta(r)$ of a vortex unit circulation at the point $R$ on the sites of the dual lattice. The source field
\( n(R) \) is \( \sum_i n_i \delta(R - R_i) \) where \( n_i \) is the quantized circulation of the vortex at \( R_i \). After some algebra, we obtained an expression for the energy of a configuration of phase angles in the presence of an arbitrary set of vortices \( n(R) \) in Eq. (50) of Ref. 17,

\[
\frac{H}{k_B T} = \frac{H_{sw}}{k_B T} + \frac{H_v}{k_B T},
\]

\[
\frac{H_{sw}}{k_B T} \approx \frac{1}{2} K_0(T) \int d^2 r (\nabla \phi(r))^2,
\]

\[
\frac{H_v}{k_B T} \approx -\pi K_0(T) \int_{|R - R'| > a} d^2 R d^2 R' n(R)n(R') \ln \frac{|R - R'|}{a} - \ln y_0 \int d^2 R n^2(R).
\]

We have eliminated the last term in the expression we gave in Eq. (50) of Ref. 17, which was proportional to the net charge and to \( \ln(L/a) \), because the correct expression for the energy of a nonzero net charge is actually sensitive to boundary conditions. For the case of a Coulomb gas enclosed by a conducting boundary, circular or polygonal, each charge is accompanied by image charges, which attract it to the boundary, so the \( \ln(L/a) \) should be replaced by a quantity of order unity. The same happens for the vortex gas in a superfluid. We therefore have a good reason to ignore this term.

This expression describes the classical XY magnet with the parameter \( K_0(T) \) equal to \( J/k_B T \), where \( J \) is the nearest neighbor interaction energy, and \( K_0(T) \) is \( (\hbar/m)^2 (\rho^0_s/k_B T) \) for a superfluid film; \( \rho^0_s \) is the bare superfluid mass per unit area. The parameter \( y_0 = \exp(-E_c/k_B T) \) is the vortex fugacity whose exact value turns out to be unimportant. The expression for \( H_{sw} \) ignores both the nonlinear interactions of the spin waves with one another, and their scattering by the vortices. The vortex core energy, \( E_c \), can be regarded as the contribution of the region close to the vortex core, \( r \leq a \), where the magnitude \( |\psi(r)| \) is varying rapidly and \( \mathbf{v}_s = \nabla \theta \) is very large, so that the quadratic form of the action is no longer a good description. The short distance cutoff, \( a \), can be regarded as the size of a vortex core and \( L \gg a \) is the linear size of the system.

Note that, in the planar magnet, the exchange constant \( J \) determines both \( K_0(T) \) and the fugacity \( y_0 \) so that the two parameters are actually not independent, although they are treated as independent parameters. This is convenient as the calculations involve a perturbation expansion in \( y_0(T) \) which violates the relation between the fugacity and \( K_0(T) \). This does not break the \( O(2) \) symmetry of the original problem and turns out not to affect
the quantities of interest, as treating $y_0$ as an independent variable is just altering an irrelevant variable which is known not to affect physical quantities. In 1972, Kosterlitz and Thouless did not understand Wilson’s seminal theory\textsuperscript{24,30} of critical phenomena and had no idea of the renormalization group classification of relevant, irrelevant and marginal operators, but this approach just felt right. Also, we were very influenced by the similarity to the 1D Ising ferromagnet with $1/r^2$ interactions, solved by Anderson, Yuval and Hamann.\textsuperscript{6} Both problems contain point defects with logarithmic interactions between them, and the treatment by Anderson, Yuval and Hamann also involved a fugacity and an interaction strength which scale differently, but whose initial values are related in an irrelevant fashion.

Smooth variations of the phase angle are controlled by $H_{sw}$ in Eq. (1.22) and lead to algebraic decay of the two-point correlation function,\textsuperscript{20}

$$\langle e^{i(\phi(r)-\phi(0))} \rangle \sim r^{-1/2} \pi K_0(T).$$

From this, we see that fluctuations destroy long range order in $2D$, since the magnetization $m = \langle e^{i\phi(r)} \rangle \sim L^{-1/4} \pi K_0(T)$, where $L$ is the linear size of the system. This approximation is insufficient to induce a transition to a true disordered phase in which one expects this correlation function to decay exponentially. To proceed further, we were faced with the daunting task of considering the problem with the Hamiltonian of Eq. (1.22) where $H_v$ is the Hamiltonian for a set of point vortices $\{n(R)\}$ interacting with a $\ln r$ Coulomb potential. We assume that the system has no net charge in the absence of an explicit external electrostatic potential.

We considered\textsuperscript{17} the problem of a neutral set of charges $n(R) = \pm 1$ since such charges have the largest fugacity and are the most probable, and ignored larger charges because these are less probable. We considered a pair of opposite charges, a distance $r$ apart, and concluded that they would be screened by the polarization of smaller pairs which were screened by yet smaller pairs. The main result of this paper is that there is a scale dependent dielectric constant $\epsilon(r) = K_0/K(r)$ where the force between a pair of opposite unit charges separated by $r$ is $2\pi K(r)/r$. The potential energy $U_{\text{eff}}(r)$ of this pair is

$$U_{\text{eff}}(r) = 2\pi \int_0^r dr' K(r') \frac{r'}{r'} \equiv 2\pi f(r) \ln \left( \frac{r}{a} \right),$$

and the results of Ref. 17 are equivalent to

$$K^{-1}(r) = K_0^{-1} + 4\pi^3 \frac{3}{y_0^2} \int_0^r \frac{dr'}{a} \left( \frac{r'}{a} \right)^{3-2\pi f(r')}.$$
We were unable to solve this and made an unfortunate and unnecessary approximation by replacing $f(r')$ by $K(r)$ in Eq. (1.25) and solving self-consistently for $K(r)$. This replacement of $f(r')$ by $K(r)$ was justified by the smallness of their difference, but it did lead to some strange and incorrect predictions.\(^{17}\)

In an important paper\(^59\) the approximation was shown to be unnecessary and a correct procedure given. Define a scale dependent fugacity by

$$y(r) = y_0 \left( \frac{r}{a} \right)^{2-\pi f(r)}$$

$$= y_0 \exp \left( 2 \ln \left( \frac{r}{a} \right) - \pi \frac{\int_a^r K(r') \, dr'}{r'} \right),$$

$$K^{-1}(r) = K_0^{-1} + 4\pi^3 \int_a^r \frac{dr'}{r'} y^2(r'),$$

so that, by differentiating these with respect to $\ln r$,

$$\frac{dy(r)}{d \ln r} = (2 - \pi K(r))y(r),$$

$$\frac{dK^{-1}(r)}{d \ln r} = 4\pi^3 y^2(r),$$

which are exactly the recursion relations derived earlier by one of us.\(^{41}\) However, even if we had not made our unnecessary approximation and derived these recursion relations, it is not clear that we would have known what to do with them as renormalization group equations for scale dependent coupling constants were unknown to the majority of physicists in 1972.

Kosterlitz was not happy with the results of our self-consistent calculations, and had been given a preprint of the paper by Anderson, Yuval and Hamann,\(^6\) which opened his eyes to strange ideas like scale dependent parameters, scaling and the renormalization group derived by performing a partial trace in a partition function for the 1D Ising model with $1/r^2$ interactions between spins. There seemed to be a definite connection between our 2D Coulomb gas problem of Eq. (1.22) and the domain wall representation of the 1D Ising model with $1/r^2$ interactions.\(^5,6\) This connection motivated him to spend some months reading and rereading the papers until he understood exactly what the recursion relations meant and how they were derived. This seemed like a worthwhile exercise because the method reduced the impossible task of computing the exact partition function for the $1/r^2$ Ising model to the more feasible task of deriving and solving a few differential equations, which gave most of the interesting information contained in the inaccessible partition function. If one could reduce the vortex representation of the 2D...
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The XY system of Eq. (1.22) to a few analogous differential equations, the few months of effort would be well spent. Finally, Kosterlitz was able to derive the recursion relations of Anderson et al. and, more importantly, understand the physical meaning of the mathematical manipulations involved. He was then able to apply these ideas to the problem of interest, which is the partition function of the 2D Coulomb gas,

\[ Z(K_0, y_0) = Z_0(K_0) \sum_{n=0}^{\infty} \frac{y^{2n}}{n!} \int d^2 \mathbf{R}_i \exp \left[ +\pi K_0 \sum_{i \neq j} n_i n_j \ln \left( \frac{|\mathbf{R}_i - \mathbf{R}_j|}{a} \right) \right], \]

\[ Z_0(K_0) = \int D\phi \exp \left( -\frac{K_0}{2} \int d^2 \mathbf{r} (\nabla \phi(\mathbf{r}))^2 \right). \] (1.28)

Here, \( Z_0(K_0) \) is the trivial Gaussian spin wave partition function, and, in the Coulomb gas part of the partition function, the integrations over the vortex positions \( \mathbf{R}_i \) are restricted by the hard core condition \( |\mathbf{R}_i - \mathbf{R}_j| > a \), where the short distance cut-off \( a \) can be taken as a lattice spacing or the diameter of a vortex core. It turns out that this cut-off length \( a \) is, to a large degree, arbitrary, but it cannot be set to zero before the end of the calculations. Similarly, the infrared cut-off, \( L \) the size of the system, must be kept finite until the end of the calculations to avoid unphysical divergences. We note that both infrared and ultra-violet cut-offs have clear physical interpretations in this case, and there is no temptation to take the limits \( a \to 0 \) or \( L \to \infty \) unless it is obvious that such limits make physical sense. In fact, these cut-offs appear only in the combination \( L/a \) and the appropriate limit is \( L/a \to \infty \) which has an obvious physical meaning.

The original derivation of the renormalization group equations was carried out in the most complicated way possible by integrating out the short distance degrees of freedom in the partition function of Eq. (1.28) where the lattice spacing has been rescaled by \( a \to ae^{\delta l} = a(1 + \delta l) \). At length scale \( a(l) = ae^l \) the effective interaction of a fugacity and free energy density are \( K = K(l), y = y(l), \) and \( f = f(l) \) respectively. Later work derived these recursion relations by technologically easier but more sophisticated methods.
The most straightforward method\textsuperscript{18} starts with the superfluid momentum density correlation function,

\[ C_{\alpha\beta}(\vec{q}, K_0, y_0) = \langle g^s_{\alpha}(\vec{q}) g^s_{\beta}(-\vec{q}) \rangle = A(q) \frac{q_{\alpha} q_{\beta}}{q^2} + B(q) \left( \delta_{\alpha\beta} - \frac{q_{\alpha} q_{\beta}}{q^2} \right). \]

(1.30)

Hohenberg and Martin\textsuperscript{61} showed that the renormalized or measured superfluid density \( \rho^R_s(T) \) is given by

\[ K_R(T) = \frac{\hbar^2 \rho^R_s(T)}{M_A k_B T} = \lim_{q \to 0} \left( A(q) - B(q) \right) = K_0 - 4\pi^2 K_0^2 \lim_{q \to 0} \frac{\langle n(\vec{q}) n(-\vec{q}) \rangle}{q^2}. \]

(1.31)

The vorticity–vorticity correlation function, \( \langle n(\vec{r}) n(0) \rangle \), is calculated as a power series in the fugacity \( y_0 \) and, to lowest order, one easily obtains

\[ K^{-1}_R(l) = K^{-1}_0 + 4\pi^3 y_0^2 \int_a^\infty \frac{dr}{a} \left( \frac{r}{a} \right)^{3-2\pi K_0} + \mathcal{O}(y_0^4), \]

(1.32)

which is essentially identical to Eq. (1.25) obtained from the self-consistent theory.\textsuperscript{59} The perturbative treatment makes explicit that this is correct to lowest order in the vortex fugacity \( y_0 \). The RG equations are obtained from Eq. (1.32) by writing

\[ \int_a^\infty = \int_a^{a(1+\delta l)} + \int_{a(1+\delta l)}^\infty, \]

(1.33)

and defining a rescaled fugacity \( y(l + \delta l) \) and interaction \( K(l + \delta l) \) by

\[ y(l + \delta l) = (2 - \pi K(l)) y(l) \delta l, \]

\[ K^{-1}(l + \delta l) = K^{-1}(l) + 4\pi^3 y^2(l) \delta l, \]

(1.34)

where \( K(l) \) and \( y(l) \) are the coupling constant and fugacity at scale \( l \), when the cut-off \( a \) has been rescaled to \( ae^l \). At this scale, the effective Hamiltonian of the system \( \mathcal{H}(K(l), y(l)) \) of Eq. (1.22) describes fluctuations on length scales larger than \( ae^l \) while the original physical Hamiltonian \( \mathcal{H}(K_0, y_0) \) describes fluctuations on all scales larger than \( a \). This is precisely Wilson’s renormalization group idea\textsuperscript{24,30} as applied to the two-dimensional Coulomb gas. Writing Eq. (1.34) as a pair of differential equations, we obtain the recursion relations

\[ \frac{dK^{-1}(l)}{dl} = 4\pi^3 y^2(l) + \mathcal{O}(y^4), \]

\[ \frac{dy(l)}{dl} = (2 - \pi K(l)) y(l) + \mathcal{O}(y^3). \]

(1.35)
which are identical to those of Eq. (1.27) except that this treatment explicitly displays that the recursion relations are a perturbation expansion in the fugacity \( y(l) \). This derivation, using the renormalized stiffness constant \( K_R \), has the big advantage that the RG equations are derived using the perturbation expansion of \( K_R(K, y) \), so that one can immediately write the exact relation,

\[
K_R(K_0, y_0) = K_R(K(l), y(l)).
\]  

(1.36)

This is a disguised version of the Josephson scaling relation\(^6\) which, in \( d \) dimensions, reads

\[
K_R(K_0, y_0) = e^{(2-d)l} K_R(K(l), y(l)).
\]  

(1.37)

All the physics of the transition is contained in Eqs. (1.35) and (1.36) and we now have to solve these simple differential equations. It is clear that transition occurs at the fixed point \( y(l) = 0 \) and \( \pi K(l) = 2 \), so we write \( \pi K(l) = 2 + x(l) \) so that, to lowest order in \( x(l) \) and \( y(l) \), Eq. (1.35) becomes

\[
\frac{dx}{dl} = -16\pi^2 y^2,
\]  

\[
\frac{dy}{dl} = -xy.
\]  

(1.38)

The solutions \( x(l) \) and \( y(l) \) are related by

\[
x^2(l) - 16\pi^2 y^2(l) = C(t),
\]  

(1.39)

where \( C(t) \) is a constant of integration, which depends on \( t = (T - T_c)/T_c \). As the scale \( l \) increases, \( x(l) \) and \( y(l) \) sweep out a set of hyperbolae in the \( y > 0 \) half plane. Physically, since \( y \) is the vortex fugacity, the density of vortices is proportional to \( y \) and \( y < 0 \) is unphysical. We identify the line \( y = 0 \) as the spin wave phase since there are no vortices or dislocations in the system if \( y = 0 \). This phase has finite rigidity and is identified as the low \( T \) ordered phase. On the other hand, a finite fugacity \( y \) implies a finite density of free defects in the system, which means that the rigidity vanishes at long length scales. We identify this situation as a high temperature disordered phase.

Having identified the possible behaviors of the system by physical arguments, it remains to demonstrate that the renormalization group flows of Eq. (1.35) and the approximate form of Eq. (1.38) yield this expected behavior. The integration constant \( C(t) \) can be taken to be zero at \( T = T_c \) and it is straightforward to convince oneself that the \( x, y \) plane splits into three different regions: (I) \( C(t) \geq 0 \), \( x(l) \geq 4\pi y(l) \geq 0 \), (II) \( C(t) < 0 \),
$|x(l)| < 4\pi y(l)$, and (III) $C(t) > 0$, $x(l) < 0$, $|x(l)| \geq 4\pi y(l)$. Regions (I)–(III) require separate solutions of Eq. (1.38). We choose $C(t) = -b^2 t$ where $t = (T - T_c)/T_c$ is the fractional deviation of $T$ from $T_c$. This linear approximation for the constant $C$ is adequate for $|t| \ll 1$ as there is every reason to expect that $C(t)$ is an analytic function of $t$ and that, to lowest order in $t$, it is linear. We identify $C(t) = 0$ as corresponding to $T = T_c$ because the trajectories $x(l; C)$ and $y(l; C)$ behave differently in the three regions.

In region I, $x(l) > 0$ and $C(t) > 0$, and we have

\[
\frac{dx}{dl} = -16\pi^2 y^2, \\
\frac{dy}{dl} = -xy,
\]

\[
x^2 - 16\pi^2 y^2 = C > 0 \Rightarrow \int_{x_0}^{x(l)} dx \left( \frac{1}{x - \sqrt{C}} - \frac{1}{x + \sqrt{C}} \right)
\]

\[
= -2l\sqrt{C},
\]

\[
x(l) = \sqrt{C} \frac{x_0 + \sqrt{C} + (x_0 - \sqrt{C})e^{-2l\sqrt{C}}}{x_0 + \sqrt{C} - (x_0 - \sqrt{C})e^{-2l\sqrt{C}}}. \tag{1.40}
\]

To examine the behavior of $x(l)$ in various limits, we can take the deviation from $T_c$ extremely small so that $x_0 \gg \sqrt{C}$ and $2l\sqrt{C} > 1$ or $2l\sqrt{C} < 1$ in different regimes which allows us to define a correlation length $\xi_-(t)$ separating the regimes. We have

\[
\xi_-(t) = e^{1/2\sqrt{|t|}} = e^{1/2b\sqrt{|t|}},
\]

\[
x(l) = \frac{x_0}{1 + x_0l} \text{ for } l \ll \xi_-(t). \tag{1.41}
\]

For $l \gg \xi_-(t)$, we immediately see that

\[
x(l) = \sqrt{C} \left( 1 + 2e^{-2l\sqrt{C}} \right) \text{ and } y(l) = \frac{\sqrt{C}}{2\pi} e^{-l\sqrt{C}}. \tag{1.42}
\]

This result gives the behavior of the renormalized stiffness constant $K_R(T)$ when $T$ is slightly below $T_c$. From Eq. (1.36), we have

\[
K_R(T) = K_R(K(l), y(l)) = K_R(K(\infty), 0)
\]

\[
= K(l = \infty) = \frac{2}{\pi} + b|t|^{\nu}, \tag{1.43}
\]

with $\nu = 1/2$. Here, we have used $y(\infty) = 0$ when the effective Hamiltonian is a Gaussian with coupling constant $\pi K(\infty) = 2 + x(\infty) = 2 + \sqrt{C}$, from
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Thus, we can deduce the behavior of the measurable stiffness constant $K_R(T)$ in the whole region, $T \leq T_c$. For $T \ll T_c$, we expect that $K_R(T)$ will decrease linearly from its $T = 0$ value as $T$ increases until a few percent below $T_c$. At this temperature, we expect that vortex fluctuations will have some effect and, in the final approach to $T_c$, the stiffness $K_R(T)$ plumbs to its universal value of $2/\pi$ as $\sqrt{|t|}$.\(^{18}\)

In region II, $x(l)$ can have either sign and $C(t) = -b^2 t < 0$, so that

$$16\pi^2 y^2 = (x^2 + |C|),$$

$$-l = \int_{x_0}^{x(l)} \frac{dx}{x^2 + |C|} = |C|^{-1/2} \left( \tan^{-1} \left( \frac{x(l)}{\sqrt{|C|}} \right) - \tan^{-1} \left( \frac{x_0}{\sqrt{|C|}} \right) \right).$$

(1.44)

Here, one chooses the upper limit of integration to be at $l$ so that $x(l) = -x_0$, and we note that we can choose the deviation from $T_c$ such that $\sqrt{|C(t)|} = b\sqrt{t} \ll x_0$, so that Eq. (1.44) reads $l = \pi |C(t)|^{-1/2}$, from which we can define a correlation length

$$\xi_+(t) = e^{\pi/b\sqrt{t}}, \quad \xi_-(t) = e^{1/2b\sqrt{t}}.$$  

(1.45)

This theory of the 2D planar rotor model and of a superfluid film has two length scales $\xi_-(t)$ and $\xi_+(t)$, both diverging exponentially at the critical point. The length scales $\xi_-$ and $\xi_+$ can be interpreted as controlling the distribution of the defects or vortices in the system. At low $T$, neutral pairs of equal but opposite vorticity are bound together as neutral pairs and the length scale $\xi_-(t)$ is interpreted as the maximum size of a vortex pair. From Eq. (1.42), the density of vortex pairs separated by more than $\xi_-(t)$ is essentially zero since the fugacity $y(l)$ is essentially zero for $e^l > \xi_-(t)$ and is identically zero when $l \to \infty$. We can interpret the absence of unbound vortices as the low $T$ phase where the phase of the complex order parameter has a finite stiffness to twists. This is analogous to a finite spring constant. Diverging correlation lengths at continuous transitions were already well known and accepted, but this exponential divergence was not known to most physicists in the early 1970’s, although, for the exactly soluble F model limit of the eight vertex model,\(^{63,64}\) the correlation length displays a similar exponential divergence.

Finally, in region III, where $C > 0$ and $x(l) = -|x(l)| < 0$, we can integrate the recursion relations exactly as for region I, except we obtain

$$|x(l)|^2 - 16\pi^2 y^2 = C,$$

$$\frac{d|x|}{dl} = |x|^2 - C.$$  

(1.46)
Since \(|x(l)| \geq \sqrt{C}\), this means that \(|x(l)|\) increases with \(l\) and, when \(|x(l)| \gg \sqrt{C}\),

\[
|x(l)| = \frac{|x(l^*)|}{1 - |x(l^*)|(l - l^*)}
\]  

(1.47)

where \(l^*\) is the value of \(l\) where the trajectory becomes indistinguishable from that with \(C = 0\). Note that the physical interpretation of a system in region III is somewhat obscure and this region is unphysical as it is not accessible for the 2D planar rotor model. The RG flows for initial Hamiltonians in this region are attracted to the line \(x(l) + 4\pi y(l) = 0\) and flow to large \(y(l)\), just as trajectories in region II. We assume that all initial Hamiltonians in regions II and III flow to the same disordered fixed point and that all the Hamiltonians correspond to the same high \(T\) disordered phase.

It appears that the system behaves differently if the initial Hamiltonian defined by parameters \(K_0(T)\) and \(y_0(T)\) lies in region I, II or III. It is clear that region I can be interpreted as a low temperature ordered phase since the vortex fugacity \(y(l)\) flows to zero as the length scale, parametrized by \(l\), increases. This means that the vortex fugacity \(y(l)\) vanishes as \(l \to \infty\) which is interpreted to mean that the system contains no free, unbound vortices at length scales larger than \(\xi_-(T)\) which, in turn, means that the measured stiffness constant can be computed in region I by exploiting Eq. (1.36) where we have used Eq. (1.39) to obtain \(x(\infty) = \sqrt{C(t)} = b\sqrt{|t|}\). In region II, it is natural to assume that \(K_R(t > 0) = 0\) which can be derived by treating the unbound vortices on scales \(e^l \gg \xi_+(t)\) by Debye–Hückel theory. Note that Eq. (1.36) predicts that the ratio \(\rho_s^R(T)/T\) has a finite and universal value at \(T_c^{-18}\)

\[
\frac{\rho_s^R(T_c^{-})}{T_c} = \frac{2MA^2k_B}{\pi\hbar^2}
\]

(1.48)

which has the approximate value \(3.491 \times 10^{-9}\) g cm\(^{-2}\)K\(^{-1}\) for liquid helium.

This result has been verified experimentally to about 10% accuracy, by measuring the variation with temperature of the moment of inertia of a cylindrical roll of Mylar film coated with a film of liquid helium. At high temperatures the normal liquid rotates as the Mylar film rotates, but at low temperatures the superfluid component of the liquid helium ceases to move with the substrate. This method of measuring superfluid density was developed in the middle of the last century by Andronikashvili. The universal jump in superfluid density of Eq. (1.48) is an inescapable prediction of the theory. If experiment had produced a different number, then the whole structure of the vortex theory would be proved incorrect and theorists would have
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been back to the drawing board. As a historical note, Bishop and Reppy performed the measurements of the superfluid density of their $^4$He films without knowledge of the theoretical prediction, and, without knowledge of the theoretical value, they measured the universal slope $\rho_s^R(T_c)/T_c$. Of course, measuring the superfluid density is not as straightforward as it appears. An important feature of this, or almost any other conceivable experiment, is that to get enough sensitivity to distinguish the moment of inertia of the helium film from that of the Mylar substrate it is necessary to use a significantly high frequency for the measurement, which was 2500 Hz in this experiment, and so the static theory described in this section is inadequate. A nonzero frequency theory was developed by Ambegaokar, Halperin, Nelson and Siggia (AHNS). This and related experiments are discussed in more detail in Sec. 1.7.1.

To show that $\rho_s^R = 0$ for $T > T_c$, we follow the treatment of Nelson by defining the generalized stiffness constant at finite $q$ as

$$K_R(q, K, y) = K_0 - 4\pi^2 K_0^2 \frac{\langle n(q) n(-q) \rangle}{q^2}.$$  (1.49)

We can use Eq. (1.37) to write

$$K_R(q, K, y) = K_R(qe^l, K(l), y(l))$$  (1.50)

up to the scale $e^l = \xi_+$ to obtain

$$K_R(q, K, y) = K(l^*) - \frac{4\pi^2 K^2(l^*)}{(qe^l)^2} \langle n(qe^l) n(-qe^l) \rangle$$  (1.51)

where the average must be calculated with the Coulomb gas ensemble with couplings $K(l^*)$ and $y(l^*)$. The vortex Hamiltonian is given by

$$\frac{H_V(l^*)}{k_B T} = \frac{1}{2} \int d^2 k \left( \frac{4\pi^2 K(l^*)}{k^2} + B(l^*) \right) n(k) n(-k).$$  (1.52)

Now, we can choose $e^l = \xi_+(T)$ at which scale the system has a dense set of vortices with all integer values of $n(r)$. In such a case, it is a reasonable approximation to integrate rather than sum over $n(q)$ when evaluating the expectation value

$$\langle n(q\xi_+) n(-q\xi_+) \rangle_{l^*} = \frac{1}{4\pi^2 K(l^*)/(q\xi_+)^2 + B(l^*)}.$$  (1.53)

Note, $B(l^*) \approx -\ln y(l^*) = \mathcal{O}(1)$ but the exact value is not important. Using this in Eq. (1.49), we obtain

$$K_R(q, T) = \frac{B(l^*) K(l^*)}{B(l^*) + 4\pi^2 K(l^*)/(q\xi_+)^2} \sim (q\xi_+)^2,$$  (1.54)

as $q\xi_+(T) \to 0$. This shows that $K_R(T) = 0$ when $T > T_c$, as expected.
Other thermodynamic quantities can be calculated from the renormalization group equations, especially when $T \leq T_c$ because the system is mapped into a simple Gaussian model when the vortex fugacity $y(l) \to 0$. For example, the two-point correlation function $G(r, K, y)$ was computed at $T_c$ by Kosterlitz\cite{Kosterlitz} who found that,

$$G(r, K, y) = \langle e^{i(\theta r - \theta(0))} \rangle \sim r^{-1/4}(\ln r)^{1/8},$$

(1.55)

when $T = T_c$. An improved derivation is sketched below from the renormalization group equations. First, we note the identity, for $d = 2$,

$$\frac{\partial G(l)}{\partial l} = \eta(l)G(l) \quad \text{where} \quad \eta(l) = \frac{1}{2\pi K(l)} = \frac{1}{4} - \frac{x(l)}{8} + O(x^2),$$

(1.56)

where

$$G(0) = G(l)\exp\left(-\int_0^l \eta(l')dl'\right)$$

We want the correlation function $G(r, K, y)$ in terms of the physical coupling constants. To use the above equation, we need to know the correlation function $G(l)$ which is calculated from the scaled parameters $K(l)$ and $y(l)$. Since our recursion relations are valid as long as the vortex fugacity $y(l)$ remains small, we can choose $l$ in Eq. (1.56) at our convenience. A sensible choice is $re^{-l} = 1$, so we need $G(re^{-l} = 1, K(l), y(l)) = O(1)$ and the singular part of the correlation function is just

$$G(r, K, y) = \exp\left(-\int_0^{\ln r} \eta(l)dl\right).$$

(1.57)

To evaluate this, we use $\eta(l) = 1/(2\pi K(l)) = 1/4 - x(l)/8 + O(x^2(l))$ where $x(l)$ is given by Eq. (1.42) and we obtain

$$\int_0^l dl'x(l') = \sqrt{C}l + \ln\left[\frac{1 - ae^{-2\sqrt{C}l}}{1 - a}\right] \quad \text{where} \quad a = \frac{x_0 - \sqrt{C}}{x_0 + \sqrt{C}} = 1 - \frac{2\sqrt{C}}{x_0},$$

$$\approx \sqrt{C}l + \ln(1 + x_0l) \quad \text{when} \quad l \ll \frac{1}{2\sqrt{C}} = \ln \xi_-(T),$$

$$\approx \sqrt{C}l + \ln \frac{x_0}{2\sqrt{C}} \quad \text{when} \quad l \gg \frac{1}{2\sqrt{C}} = \ln \xi_-(T).$$

(1.58)

Thus, for $T \leq T_c$, we obtain

$$G(r, t) \sim r^{-\eta(T)}(\ln r)^{1/8} \quad \text{when} \quad 1 \ll r \ll \xi_-(t),$$

$$G(r, t) \sim r^{-\eta(T)} \quad \text{when} \quad 1 \ll \xi_-(t) \ll r,$$

(1.59)
where $\eta(T) = 1/(2\pi K_R(T))$. Note that, when $r \gg \xi(t)$, a pure power law decay with a temperature dependent exponent, $\eta(T) = 1/(2\pi K_R(T))$, is obtained, corresponding to an effective Gaussian model with a renormalized coupling constant $K_R(T) = K(l = \infty)$. For $r \ll \xi(t)$, we obtain the same power law decay with a temperature dependent exponent, $\eta(T) = 1/(2\pi K_R(T))$, corresponding to an effective Gaussian model with a renormalized coupling constant $K_R(T) = K(l = \infty)$.

The forms of $G(r,t)$ of Eq. (1.59) are true for $t \leq 0$ for all values of $r$, and also for $t > 0$ when $r < \xi(t)$. However, above $T_c$, we expect that the correlation function $G(r,t) \sim \exp(r/\xi(t))$ when $r \gg \xi(t)$. To show this, we have to be more careful in our use of the RG equation, Eq. (1.56). In this situation, we must choose $l^* = \ln \xi(t)$ because this is the limit of validity of the recursion relations, and we obtain

$$G(r,K,y) = G(r/\xi(t),K(l^*),y(l^*)) \exp \left( -\int_0^{l^*} dl \eta(l) \right).$$

Equation (1.60) summarizes the content of our RG equations, relating the correlation function of the original system to the correlation function, $G(r/\xi(t))$, of an effective system where the minimum length scale is $\xi(t)$, but at a very high temperature. An explicit calculation was done in Ref. 60, using a duality transformation, to obtain the expected result for $r \gg \xi(t)$,

$$G(r,t) \sim \exp \left( -\frac{r}{\xi(t)} \right).$$

1.6. Scaling Theory in Analogous Systems

1.6.1. Duality and the roughening of crystal facets

Interestingly, and it surprised us, the $2D$ planar rotor model is intimately related to models for the roughening of equilibrium crystal facets as the temperature $T$ is varied. This analogy was pointed out by Chui and Weeks.\textsuperscript{74,75} The lattice points of an ideal facet are represented as a two-dimensional lattice, and smooth deviations away from the ideal lattice can be represented as a function of the position on the ideal facet.

If the equilibrium state of a given crystal facet is a smooth plane, that facet may appear in a crystal grown at this temperature, but it is also possible that a stable facet may not occur because it grows too slowly in comparison with competing facets. In particular, it has been known for a long time that a crystal face with screw dislocations in it may grow much faster.
than an ideal crystal face. There has been a hope that quantum crystals, such as solid $^4$He surrounded by the superfluid liquid, may equilibrate fast enough for the equilibrium facets to appear.

It is not difficult to see that the partition function of the 2D Coulomb gas representation of the 2D planar rotor model of Eq. (1.22) can be written as

$$Z(K, y) = \sum_{n(r)} \exp \left( -2\pi^2 K \sum_{\mathbf{r}, \mathbf{r}'} G(\mathbf{r}, \mathbf{r}') n(\mathbf{r}) n(\mathbf{r}') - \ln \sum_{\mathbf{r}} n^2(\mathbf{r}) \right)$$

$$= \sum_{n(r)} \left( \prod_{\mathbf{r}} \int_{-\infty}^{+\infty} \frac{d\phi(\mathbf{r})}{2\pi} \right) \exp \left( -\frac{1}{2K} \sum_{\mathbf{r}, \mathbf{r}'} (\phi(\mathbf{r}') - \phi(\mathbf{r}))^2 + 2\pi i \sum_{\mathbf{r}} n(\mathbf{r}) \phi(\mathbf{r}) - \ln \sum_{\mathbf{r}} n^2(\mathbf{r}) \right),$$

where

$$G(\mathbf{r}, \mathbf{r}') = \int \frac{d^2 q}{(2\pi)^2} e^{i\mathbf{q} \cdot \mathbf{r} - \mathbf{r}'} = \frac{1}{2\pi} \ln | \mathbf{r} - \mathbf{r}' |. \quad (1.62)$$

At this point, we can make the approximation for the vortex fugacity of $y = 1$ and $\sum_{-\infty}^{+\infty} e^{2\pi i \phi} = \sum_{-\infty}^{+\infty} \delta(\phi - \hat{h})$ when we obtain the discrete Gaussian model, or we can take $y \ll 1$ so that the partition function becomes

$$Z(K, y) = \int \prod_{\mathbf{r}} \frac{d\phi(\mathbf{r})}{2\pi} \exp \left[ -\frac{1}{2K} \sum_{\mathbf{r}, \mathbf{r}'} (\phi(\mathbf{r}) - \phi(\mathbf{r}'))^2 \right] [1 + 2y \cos(2\pi \phi(\mathbf{r}))]$$

$$= \int \prod_{\mathbf{r}} \frac{d\phi(\mathbf{r})}{2\pi} \exp \left[ -\frac{1}{2K} \sum_{\mathbf{r}, \mathbf{r}'} (\phi(\mathbf{r}) - \phi(\mathbf{r}'))^2 + 2y \sum_{\mathbf{r}} \cos(2\pi \phi(\mathbf{r})) \right]. \quad (1.63)$$

The last step to convert this into the sine-Gordon roughening model is to define the height variable by $\phi(\mathbf{r}) = h(\mathbf{r})/b$ where $h(\mathbf{r})$ is the local facet height above a reference plane in steps of the interplane distance $b$. We finally obtain the sine-Gordon representation of the roughening problem as

$$H(\gamma, u) = H_0 + H_u = \frac{\gamma}{2} \int d^2 \mathbf{r} (\nabla h(\mathbf{r}))^2 - u \int \frac{d^2 \mathbf{r}}{a^2} \cos \left[ \frac{2\pi h(\mathbf{r})}{b} \right], \quad (1.64)$$

where $u = 2y$ when $y \ll 1$ and $a$ is the short distance cut off.

One can derive renormalization flow equations for the parameters $\gamma(l)$ and $u(l)$ in a similar way to $K(l)$ and $y(l)$ in the vortex system by defining
a renormalized surface stiffness $\gamma_R(T)$ as,

$$F(v) - F(0) = \frac{1}{2} \Omega \gamma_R(T) v^2,$$

$$v = \frac{1}{\Omega} \int d^2r \langle \nabla h(r) \rangle,$$

(1.65)

where $F(v)$ is the free energy of a surface of area $\Omega$, and $v$ is the average gradient of $h(r)$. Writing $h(r) = v \cdot r + h'(r)$, the sine-Gordon Hamiltonian is

$$H(v) = \frac{1}{2} \Omega v^2 + H_0[h'(r)] + H_u[h'(r) + v \cdot r].$$

(1.66)

Expanding $F(v) = -k_B T \ln \text{Tr} \exp(-H(v)/k_B T)$ to $O(v^2)$, we obtain

$$\gamma_R(T) = \gamma + \frac{1}{2\Omega} \sum_{\alpha \beta} \frac{\partial^2}{\partial v_\alpha \partial v_\beta} \left( \langle H_u \rangle_0 - \frac{1}{2k_B T} \langle \langle H_u \rangle_0 - \langle H_u \rangle_0^2 \rangle \right) + \cdots$$

$$= \gamma + \frac{k_B T}{8} \left( \frac{2\pi}{b} \right)^2 u^2 \int \frac{d^2r}{a^2} \left( \frac{v}{a} \right)^2 \langle \cos \left[ \frac{2\pi}{b} (h'(r) - h(0)) \right] \rangle_0,$$

(1.67)

where $K = k_B T/(\gamma b^2)$ and we have used $\langle \cos [(2\pi/b)(h(r) - h(0))] \rangle_0 = (r/a)^{-2\pi K}$.

Equations (1.67) and (1.32) have identical forms, and flow equations for the parameters $K(l)$ and $u(l)$ can be written down immediately,

$$\frac{dK^{-1}}{dl} = \pi^3 u^2 + O(u^4),$$

$$\frac{du}{dl} = (2 - \pi K) u + O(u^3).$$

(1.68)

The only difference is in the temperature, $T$, dependence of the parameter $K(T)$. For the roughening model, $K(T) = k_B T/(\gamma b^2)$, while for the $^4$He film, $K(T) = (h/m)^2 \rho_0/(k_B T)$. This inversion of the temperature is to be expected because the roughening model is dual to the planar rotator model, and the low $T$ phase of one becomes the high $T$ phase of the other. Thus, in the high $T$ phase of the roughening model, the parameter $u(l)$ → 0, and the Hamiltonian becomes $H/(k_B T) = (K_R(T)/2) \int d^2r (\nabla h)^2$. The integer spacing between the crystal planes becomes irrelevant at large scales and the interface becomes rough. For $T < T_R$, where $T_R$ is the roughening temperature, the parameter $u(l)$, which is analogous to the fugacity $y(l)$, is relevant, leading to a flat or faceted interface.
Another result from the planar rotor model, which can be directly taken over to the roughening case, is the universal relation,

\[ K_R(T_R^+) = \frac{k_B T_R}{\gamma_R(T_R^+) b^2} = \frac{2}{\pi}. \] (1.69)

This result, which follows directly from our results for the planar rotor model and duality, implies that facets with the largest lattice spacing \( b \) will have the highest roughening temperature \( T_R \), assuming that the surface stiffness \( \gamma \) does not depend strongly on \( b \). To convert these theoretical predictions into terms of measurable quantities, we must remember that these facets are faces of a finite 3D crystal, so the equilibrium theory of a crystal of fixed volume is needed. The basic idea is that the crystal shape is determined by the condition that the total surface free energy be minimized at fixed total volume.\(^{76}\) A flat facet with coordinate \(-x_0 \leq x \leq +x_0\), in terms of reduced coordinates \( \tilde{x} = x/L, \tilde{y} = y/L \) and \( \tilde{h} = h/L \), obeys

\[
\tilde{h}(\tilde{x}, 0) = \tilde{h}_0 - A(|\tilde{x}| - \tilde{x}_0)^{3/2} \quad \text{for} \quad |\tilde{x}| > \tilde{x}_0,
\]

\[
\tilde{h}(\tilde{x}, 0) = \tilde{h}_0 \quad \text{for} \quad |\tilde{x}| < \tilde{x}_0,
\] (1.70)

where the reduced facet size, \( \tilde{x}_0 \sim b/\xi(t) \sim \exp(-B/\sqrt{|T - T_R|}) \), and \( \tilde{h}_0 = f_0/\gamma \), with \( f_0 \) the free energy per unit area of the facet.

For \( T > T_R \), the facet has disappeared and the reduced interface height is,

\[
\tilde{h}(\tilde{x}, 0) = \tilde{h}_0 - \frac{\gamma}{2\gamma_R} \tilde{x}^2,
\] (1.71)

so that the curved rough surface has a reduced curvature, \( K_R(T) = (L/R)(k_B T/\gamma_R b^2) = 2/\pi \), at \( T = T_R^+ \), which jumps discontinuously to zero at \( T = T_R^- \). Here, \( L \) is the system size and \( R \) is the radius of curvature.\(^{76,77}\) This is the analogue of the universal jump in the superfluid density \( \rho_s(T_c^-)/T_c \) in a 2D superfluid film. Of course, measuring this predicted jump in the reduced curvature of a disappearing facet is not easy and, to the best of our knowledge, the universal predictions have not yet been experimentally verified, particularly that the facet size vanishes as \( \xi^{-1}(T) \),\(^{73,78}\) but our speculation is that the discrepancy is due to lack of equilibration of the crystal.

### 1.6.2. Substrate effects

The development of the theory was motivated mainly by some very early experiments on thin films of \(^4\text{He} \) adsorbed on a substrate. This system is directly related to the 2D \( XY \) model and the predictions for the latter are
directly applicable to $^4$He films, provided one can argue that the substrate has no effect or is irrelevant in the RG sense. Substrates are essential for any two-dimensional system as it cannot exist without being supported by a substrate. To our knowledge, the only systems which do not need to be supported everywhere are thin films of liquid crystals and a monolayer of graphene, since these are sufficiently strong to survive being suspended from two edges. An isolated thin film of $^4$He or of a magnet cannot exist in the absence of a substrate. In view of this, it is vital to assess the effect of possible perturbations due to a substrate on the ideal two-dimensional system of Sec. 1.5. Before discussing the important effects of the substrate on 2D $XY$ systems, we can immediately see why experiments on superfluidity in $^4$He films can be understood in terms of the idealized theory of Sec. 1.5. This ignores the far from perfect Mylar substrate which can be modeled by a random potential coupling to the local film density $|\psi(r)|^2$. Since the order parameter field is the quantum mechanical condensate wave function, $\psi(r) = |\psi(r)|e^{i\theta(r)}$, the substrate potential cannot couple to the phase of the condensate wave function but only to its amplitude and is, thus, irrelevant. This argument justifies the use of the ideal theoretical model for superfluid $^4$He films, and partly explains why theoretical predictions agree so well with experiments.

Many other systems are influenced by the substrate, an example being a magnetic system which is heavily influenced by crystal fields with the symmetry of the substrate crystal structure. Consider a 2D $XY$ ferromagnet on a periodic lattice described by a Hamiltonian,

$$\beta H = \frac{1}{2}K(T) \int d^2r (\nabla \theta)^2 - h_p \int d^2r \cos(p\theta),$$

where $h_p$ is the strength of the $p$-fold symmetry breaking field. This sort of symmetry breaking term represents a crystal field in an $XY$ magnet, and its significance is immediately seen when $|h_p| \gg 1$ in Eq. (1.72). For $h_p > 0$, the free energy is minimized when $\cos p\theta(r) = +1$ or $\theta(r) = 2n\pi/p$ and, when $h_p < 0$, $\theta(r) = (2n + 1)\pi/p$, where $n = 0, 1, \ldots, p - 1$. These models are known as $p$-state clock models and correspond to the very well known nearest neighbor Ising ferromagnet when $p = 2$ and to the 3-state Potts model for $p = 3$. For larger values, $p = 4, 5, \ldots$, there are many variants depending on the strengths and signs of the higher harmonics of the anisotropy, $\cos[np\theta(r)]$, and of the interaction on a lattice,

$$\beta H = \sum_{(r,r')} \sum_{n=1}^{[p/2]} K_n [1 - \cos(n(\theta(r) - \theta(r')))] - \sum_{r} \sum_{n=1}^{[p/2]} h_{pn} \cos(n p \theta(r)).$$
Remarkably, one can show that this Hamiltonian contains many models in two dimensions which have been of great interest in statistical mechanics, such as the Ising model, various clock models, the $p$-state Potts models, etc. For example, the 4-state Potts model is obtained when $h_4 \to \infty$ which restricts $\theta(r) = 0, \pi/2, \pi, 3\pi/2$ and $K_1 = 2K_2$. There exists an extensive literature on the connections between these models and the Coulomb gas representations of Eq. (1.73).\textsuperscript{82–85}

In the simplest case with only the $n = 1$ terms in Eq. (1.73), we can replace the term in the partition function,\textsuperscript{86}

$$e^{hp \cos \theta} \to \sum_{m=-\infty}^{+\infty} e^{ipm\theta} e^{(ln y_p)m^2},$$

where $y_p \approx h_p/2$, so that the Coulomb gas representation of the partition function for an XY model in a $p$-fold symmetry breaking field becomes\textsuperscript{60}

$$Z \propto Z_c (K, y, y_p) = \sum_{n(R)} \sum_{m(r)} e^{-\mathcal{H}_c},$$

$$\mathcal{H}_c = \pi K_0(T) \sum_{R, R'} n(R)n(R') \ln \left( \frac{|R - R'|}{a} \right) + \ln y \sum_{R} n^2(R)
+ \frac{p^2}{4\pi K} \sum_{r, r'} m(r)m(r') \ln \left( \frac{|r - r'|}{a} \right) + \ln y_p \sum_{r} m^2(r)
+ ip \sum_{R, r} n(R)m(r) \tan^{-1} \left( \frac{Y - y}{X - x} \right).$$

Here, the integer vortices $n(R)$ lie on the dual lattice with sites at $R = (X, Y)$, and the symmetry breaking charges $m(r)$ are on the original lattice with sites at $r = (x, y)$. Both $n(R)$ and $m(r)$ obey neutrality constraints $\sum_R n(R) = 0 = \sum_r n(r)$ and the two Coulomb gases are coupled by the angular factor $ip\Theta(R - r)$. Interestingly, Eq. (1.75) shows a remarkable duality relation\textsuperscript{60} under the relabeling of the summation variables $n(R) \leftrightarrow m(r)$, the replacements $y \leftrightarrow y_p$, and $K \leftrightarrow p^2/(4\pi^2K)$ the partition function is unchanged, so that

$$Z(K, y, y_p) = Z \left( \frac{p^2}{4\pi^2K}, y_p, y \right).$$
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It is straightforward to write down the recursion relations as expansions in the fugacities $y$ and $y_p$ which read, to lowest order,

\[
\frac{dK^{-1}}{dl} = 4\pi^3 y^2 - \pi p^2 K^{-2} y_p^2,
\]

\[
\frac{dy}{dl} = (2 - \pi K) y,
\]

\[
\frac{dy_p}{dl} = \left(2 - \frac{p^2}{4\pi K}\right) y_p.
\]  (1.77)

These are consistent with the duality relation of Eq. (1.76) and were first derived from this.\[60\]

From these RG equations, we see that the charge fugacity $y_p$ is relevant at temperatures for which $K^{-1} < 8\pi/p^2$ while the vortex fugacity $y$ is relevant for $K^{-1} > \pi/2$. Thus, when $p > 4$, there is a band of temperatures,

\[
\frac{2}{\pi} \leq K_R(T) \leq \frac{p^2}{8\pi},
\]  (1.78)

for which both fugacities, $y$ and $y_p$, are irrelevant when the system reduces to a Gaussian model, and is the same as the pure XY model at low temperature. At lower temperatures, $K_R^{-1}(T) < 8\pi/p^2$, the anisotropy term $h_p\cos p\theta$ becomes relevant, the XY spins are restricted to one of $p$ directions, and the system becomes a discrete $Z_p$ clock model. Note that, for $p = 2$ and $p = 3$, there is no intermediate region where both fugacities are irrelevant, so that one expects that the model has a transition at $T_c$ in the 2D Ising class when $p = 2$, and the 3-state Potts class when $p = 3$. For the special case, $p = 4$, the multicritical point, $K = 2/\pi$ and $y = y_4 = 0$, is the meeting point of three critical lines separating a high $T$ disordered phase and two low $T$ ordered phases with two different spin orientations of $\theta(r) = n\pi/2$ or $\theta(r) = (2n+1)\pi/4$, with $n = 0, 1, 2, 3$. This point is identical to the critical point of the $F$ model,\[63\] and the three critical lines of continuously varying exponents meeting there, are in the universality class of the Baxter model.\[64\] The detailed connections with the Coulomb gas models are discussed in Refs. 82, 83 and 85. The phase diagram for models with $p \geq 5$ is similar except for a region of massless phase separating the two ordered phases from the disordered phase.\[60\]

Other interesting models of experimental relevance are obtained by including both the first and second harmonics of the $p$-fold anisotropy. The
XY model with both four- and eight-fold anisotropy terms

\[ \frac{H}{k_B T} = -K \sum_{r} \cos(\theta(r) - \theta(r')) - h_4 \sum_{r} \cos(4\theta(r)) \]

\[ + h_8 \sum_{r} \cos(8\theta(r)) \quad (1.79) \]

is interesting as a theoretical model but can also be used as a model describing the adsorption system H/W(100), hydrogen adsorbed on the (100) surface of tungsten. Changing the hydrogen coverage does not affect \( h_8 \), but drives the value of \( h_4 \) through zero, which corresponds to a structural transition of the tungsten surface.\(^{87,88}\) When \( K^{-1} \leq \pi/2 \), Eq. (1.79) has two ordered phases with finite magnetization in one of the four directions \( \theta(r) = n\pi/2 \) with \( n = 0, 1, 2, 3 \) when \( h_4 > 0 \), and \( \theta(r) = (2n + 1)\pi/4 \) when \( h_4 < 0 \). The two ordered phases are separated by a continuous transition in the universality class of the 2D XY model at \( h_4 = 0 \). The extra anisotropy term, \( h_8 \sum \cos 8\theta(r) \), is irrelevant for \( K^{-1} \geq \pi/8 \) and relevant for \( K^{-1} < \pi/8 \). Thus, in the temperature range \( \pi/8 \leq K^{-1} \leq \pi/2 \), the ordered phases will be separated by a line of continuous transitions. However, at lower temperatures, \( K^{-1} < \pi/8 \), \( h_8 \) becomes relevant and has important effects. There are two possible situations, (i) \( h_8 < 0 \) when the orderings favored by \( h_8 \) are compatible with those favored by a finite \( h_4 \), independent of the sign of \( h_4 \). In this case, the transition at \( h_4 = 0 \) between the two ordered phases will be a discontinuous first order transition.\(^{87,88}\) In case (ii), when \( h_8 > 0 \), the orderings favored by \( h_4 \) and \( h_8 \) are incompatible, resulting in an extra phase for small \( |h_4| \) with the new phase separated from the the two ordered phases by continuous Ising transitions. The first scenario is compatible with the experimental data,\(^{89,90}\) which seems to favor a first order transition at low temperature.

Another system, in which the first two harmonics of the local anisotropy potential have important effects, is tilted hexatic phases of liquid crystals. Experiments on the transitions between different tilted hexatic phases in thermotropic liquid crystals have observed a weak first order transition from the hexatic-I to hexatic-F phase.\(^{91}\) Also, in an analogous layered lyotropic liquid crystal, the \( L_\beta I \) and \( L_\beta F \) phases, corresponding to the hexatic-I and hexatic-F phases, were shown to be separated by a third \( L_\beta L \) phase with continuous Ising-like transitions between the phases.\(^{92}\) These surprising observations can be explained by coupled XY models for the bond angle, \( \theta(r) \), of the hexatic and the tilt-azimuthal angle, \( \phi(r) \), of the director with
Hamiltonian,\(^93,94\)
\[
\beta H = \int d^2r \left[ \frac{1}{2} K_6 (\nabla \theta)^2 + \frac{1}{2} K_1 (\nabla \phi)^2 + g \nabla \theta \cdot \nabla \phi + V(\theta - \phi) \right],
\]
\[
V(\theta - \phi) = -h_6 \cos(6(\theta - \phi)) - h_{12} \cos(12(\theta - \phi)) + \cdots,
\]
which is similar to Eq. (1.79). The low temperature region is the one of interest, when one can write Eq. (1.80) as,
\[
\beta H = \int d^2r \left[ \frac{1}{2} K_6 (\nabla \theta_+)^2 + \frac{1}{2} K_1 (\nabla \theta_-)^2 + V(\theta_-) \right],
\]
\[
\theta_+ = \frac{(K_6 + g)\theta + (K_1 + g)\phi}{K_6 + K_1 + 2g}, \quad \theta_- = \theta - \phi,
\]
\[
K_+ = K_6 + K_1 + 2g, \quad K_- = \frac{K_1 K_6 - g^2}{K_+}.
\]
This model system has been analyzed in detail,\(^94\) with results in accord with experiment with the various scenarios determined by the sign of the coefficient \(h_{12}\).

### 1.6.3. Melting of a 2D crystal

In our early paper\(^17\) we proposed that a two-dimensional crystal melts by the unbinding of bound pairs of dislocations which are the appropriate topological defects which destroy the translational order in a periodic crystal. It is now apparent that these physical ideas are correct but incomplete.\(^42\) A periodic crystal has two types of order (i) translational order and (ii) orientational order, and a fundamental question is: how are these orders destroyed as the temperature increases and what sort of transitions occur? The theory of 2D melting was worked out in 1978–79 in the seminal papers of Halperin, Nelson, and Young\(^42,43,95\) where it was shown that, as \(T\) is increased, there is first a dislocation unbinding transition from a low temperature crystal phase with power law decay of translational order to a fluid phase with exponentially decaying translational order, as we expected.\(^17\) The breakthrough of Halperin, Nelson and Young was to recognize the importance of the angular terms in the dislocation–dislocation interaction. We ignored these angular terms on the grounds that these are subleading. By analyzing the system carefully, they realized that the dislocation unbinding transition at \(T_m\) did not lead to an isotropic fluid, but to an intermediate anisotropic fluid phase with exponentially decaying translational order, but algebraic orientational order, due to remnants of the orientational order of the crystal. At
a higher temperature, $T_I$, the orientational order is destroyed, and the resulting high temperature phase is an isotropic fluid with exponential decay of both translational and orientational orders. Some experimental investigations and computer simulations of melting followed, but seemed to favor a direct first order transition from a solid to an isotropic fluid, in disagreement with theory which predicts two successive continuous transitions, with an intermediate partially ordered phase. At present, to our knowledge, computer simulations are unable to reproduce the theoretical predictions. Surprisingly, experiments on melting in 2D are finally in agreement with theory, but these experiments\textsuperscript{72} have been possible only over the last decade!

The notion of a crystal in 2D was somewhat controversial in 1972, when we began to think about the physics of melting because of the rigorous theorem that there is no crystalline order in two dimensions.\textsuperscript{56} This theorem is correct, but somewhat misleading, as all it shows is that true long range translational order does not exist in 2D, but it does allow for a finite elastic shear modulus in 2D, as was realized by the author of the theorem.\textsuperscript{56} We pictured a 2D elastic crystal as a periodic array of points (particles) on an elastic sheet. Then we asked: what happens to the periodic array when the sheet is elastically distorted without tearing? It is obvious that, locally, the lattice does not change much, but the relative separation of any pair of distant points can undergo a very large change. With this pictorial interpretation in mind, the idea of a 2d crystal became much clearer. We realized that the essential feature is not the translational order, but that the elastic moduli are finite. This picture is readily written in mathematical language by writing the local density, $\rho(r)$, as

\begin{equation}
\rho(r) = \rho_0(r) + \sum_G \rho_G e^{iG \cdot u(r)},
\end{equation}

where $r$ denotes the sites of the periodic reference lattice, $G$ are the reciprocal lattice vectors obeying $G \cdot r = 2\pi n$ and $u(r)$ is the displacement of the particle from its equilibrium position $r$.

The most common crystal structure in 2D is a triangular lattice in which each particle has six neighbors. There is also a six-fold rotational symmetry as the crystal axes make angles $2\pi n/6$ relative to one another. Thus, the translational and orientational order parameters are\textsuperscript{42}

\begin{equation}
\rho_G(r) = e^{iG \cdot u(r)} \quad \text{and} \quad \psi_6(r) = e^{6i\theta(r)},
\end{equation}

where $\theta(r)$ is the angle the local crystal axis makes with some arbitrary direction. Today, the natural way to proceed is to write down a Ginsburg–Landau–Wilson functional in terms of the order parameters $\rho_G(r)$ and $\psi_6(r)$,
which are invariant under the appropriate symmetry transformations. This was achieved in 1979 by Halperin, as reported by Nelson, by constructing an appropriate free energy functional in terms of the first six translational order parameters \( \rho_\alpha(\mathbf{r}) \) where \( \alpha = 1, 2, \ldots, 6 \). Following the treatment by de~Gennes for a smectic-
A–nematic transition, one obtains,

\[
F[\rho_\alpha, \theta] = \sum_{\alpha=1}^{6} \int d^2r \left( \frac{A}{2} |\mathbf{G}_\alpha \cdot \mathbf{D}_\alpha \rho_\alpha|^2 + \frac{B}{2} |\mathbf{G}_\alpha \times \mathbf{D}_\alpha \rho_\alpha|^2 + \frac{r(T)}{2} |\rho_\alpha|^2 \right) \\
+ \int d^2r \left( w(\rho_1 \rho_3 \rho_5 + \rho_2 \rho_4 \rho_6) + \frac{K_A}{2} (\nabla \theta(\mathbf{r}))^2 \right), \tag{1.84}
\]

\[
\mathbf{D}_\alpha = \nabla - i(\hat{\mathbf{z}} \times \mathbf{G}_\alpha) \theta(\mathbf{r}),
\]

where \( \mathbf{G}_\alpha \), with \( |\mathbf{G}_\alpha| = G_0 \), are the six smallest reciprocal lattice vectors of the underlying lattice, and \( \hat{\mathbf{z}} \) is a unit vector normal to the plane of the system. In the mean field approximation, the presence of third order terms in the free energy functional makes the transition first order. However, following the philosophy of the planar rotor model, we assume that the temperature, \( T \), is well below the mean field transition temperature so that \( r(T) \ll 0 \) in Eq. (1.84). This means the \( |\rho_\alpha| \) are a constant, \( \rho_0 \), so one can make the phase only approximation by writing \( \rho_\alpha(\mathbf{r}) = \rho_0 e^{i \mathbf{G}_\alpha \cdot \mathbf{u}(\mathbf{r})} \). The free energy of Eq. (1.84) is minimized when

\[
\theta(\mathbf{r}) = \frac{1}{2} (\nabla \times \mathbf{u}(\mathbf{r})), \tag{1.85}
\]

and the elastic free energy for a 2D triangular crystal is

\[
F = \frac{1}{2} \int d^2r [2\mu u_{ij}^2(\mathbf{r}) + \lambda u_{kk}^2(\mathbf{r})], \tag{1.86}
\]

where the Lamé coefficients are, in terms of \( A \) and \( B \) of Eq. (1.84) are,\(^{65}\)

\[
\mu = \frac{3}{4} \rho_0^2 (A + B) G_0^4, \quad \lambda = \frac{3}{4} (A - B) G_0^4. \tag{1.87}
\]

At quadratic order, the free energy is a functional of the linearized symmetric strain tensor,

\[
u_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i} \right). \tag{1.88}
\]

The strain field can be decomposed as \( u_{ij}(\mathbf{r}) = \phi_{ij}(\mathbf{r}) + u_{ij}^s(\mathbf{r}) \) where \( \phi_{ij}(\mathbf{r}) \) is the smooth part of \( u_{ij} \) and \( u_{ij}^s \) is the singular part due to dislocations.
which can be characterized by the amount for which the integral of the displacement \( \mathbf{u} \) round a closed contour fails to close,

\[
\oint d\mathbf{u} = a_0 \mathbf{b}(\mathbf{r}) = a_0 (n(\mathbf{r})\mathbf{\hat{e}}_1 + m(\mathbf{r})\mathbf{\hat{e}}_2). \tag{1.89}
\]

Here, \( a_0 \) is the lattice spacing, \( \mathbf{b}(\mathbf{r}) \) is the dimensionless Burger’s vector of the singularity, \( n(\mathbf{r}), m(\mathbf{r}) \) are integers, and \( \mathbf{\hat{e}}_{1,2} \) are the unit lattice vectors of the underlying triangular lattice.

Using results from linear elasticity theory, one can solve for the strain \( u^s_{ij}(\mathbf{r}) \) due to a dislocation density, \( \mathbf{b}(\mathbf{r}') = \sum_\alpha b_\alpha \delta(\mathbf{r}' - \mathbf{r}_\alpha) \), to obtain

\[
u^s_{ij}(\mathbf{r}) = \left( \frac{1}{2\mu} \epsilon_{ik} \epsilon_{jm} \frac{\partial^2}{\partial r_k \partial r_l} - \frac{\lambda}{4\mu(\lambda + \mu)} \delta_{ij} \nabla^2 \right) a_0 \sum_{\mathbf{r}'} b_m G_m(\mathbf{r}, \mathbf{r}'). \tag{1.90}
\]

The vector Green’s function, \( G(\mathbf{r}, \mathbf{r}') \), satisfies the biharmonic equation,

\[
\nabla^4 G_m(\mathbf{r}, \mathbf{r}') = -K_0 \epsilon_{mn} \frac{\partial}{\partial r_n} \delta(\mathbf{r} - \mathbf{r}'), \tag{1.91}
\]

\[
K_0 = \frac{4\mu(\mu + \lambda)}{(2\mu + \lambda)}.
\]

To solve this differential equation for \( G_m(\mathbf{r}, \mathbf{r}') \), one can consider a crystal with free boundaries which requires von Neumann boundary conditions, \( \nabla G_m(\mathbf{r}, \mathbf{r}') = \) constant, for \( \mathbf{r} \) on the boundary, so that

\[
G_m(\mathbf{r}, \mathbf{r}') = \frac{K_0}{4\pi} \epsilon_{mn} (r_n - r'_n) \left[ \ln \left( \frac{|\mathbf{r} - \mathbf{r}'|}{a} \right) + C \right]. \tag{1.92}
\]

Here, the constant \( C > 0 \) is a measure of the ratio of the core diameter to the cut-off \( a \). This can be absorbed into an effective dislocation core energy, exactly as is done for the simpler vortex case of Sec. 1.5. The final result of these tedious calculations is that the effective elastic Hamiltonian, \( H_E \), can be decomposed into a smooth part and a singular part due to dislocations as,

\[
H_E = H_0 + H_D,
\]

\[
\frac{H_0}{k_B T} = \frac{1}{2} \int \frac{d^2 \mathbf{r}}{a_0^2} (2\tilde{\mu} \phi^2_{ij}(\mathbf{r}) + \tilde{\lambda} \phi^2_{kk}(\mathbf{r})),
\]

\[
\frac{H_D}{k_B T} = \frac{K}{8\pi} \sum_{\mathbf{r} \neq \mathbf{r}'} b_\alpha(\mathbf{r}) b_\beta(\mathbf{r}') \left( \ln \left( \frac{|\mathbf{r} - \mathbf{r}'|}{a} \right) \delta_{\alpha\beta} - \frac{(\mathbf{r} - \mathbf{r})_{\alpha}(\mathbf{r} - \mathbf{r}')_{\beta}}{|\mathbf{r} - \mathbf{r}'|^2} \right) + \frac{E_c}{k_B T} \sum_\mathbf{r} |\mathbf{b}(\mathbf{r})|^2. \tag{1.93}
\]
where $K = K_0 a_0^2 / (k_B T)$, $\tilde{\mu} = \mu / (k_B T)$, and $\tilde{\lambda} = \lambda / (k_B T)$. The dislocation density is subject to the neutrality condition, $\sum \mathbf{b}(\mathbf{r}) = 0$, because the energy of an isolated dislocation diverges as $\ln L$, where $L$ is the linear size of the system.

In analogy with the 2D superfluid, we immediately conclude that the low $T$ phase of our 2D crystal is one in which there are no isolated dislocations. There will be a finite concentration of bound pairs and triplets of dislocations, which renormalize the elastic constants downwards from their bare values. The crystal is described by the Gaussian Hamiltonian $H_0$ of Eq. (1.93), which gives the Debye–Waller factor $C_G(\mathbf{r})$ and the structure function $S(\mathbf{q})$:

$$C_G(\mathbf{r}) = \langle \rho_G(\mathbf{r}) \rho_G^*(0) \rangle^0 \sim r^{-\eta_G(T)},$$

$$\eta_G(T) = \frac{k_B T |G|^2}{4\pi} \frac{3\mu + \lambda}{\mu(2\mu + \lambda)},$$

(1.94)

$$S(\mathbf{q}) = \langle |\rho(\mathbf{q})|^2 \rangle = \sum_\mathbf{r} e^{i\mathbf{q} \cdot \mathbf{r}} \langle e^{i\mathbf{q} \cdot [\mathbf{u}(\mathbf{r}) - \mathbf{u}(0)]} \rangle \sim |\mathbf{q} - \mathbf{G}|^{-2 + \eta_G(T)}.$$  

This means that there is no long range translational order in a 2D crystal because $\langle \rho_G(\mathbf{r}) \rangle = 0$, in agreement with the Mermin–Wagner theorem, but the harmonic crystal has a finite shear modulus $\tilde{\mu}(T) > 0$. Interestingly, the structure function $S(\mathbf{q})$ diverges at a set of small reciprocal lattice vectors $\mathbf{G}$ when $\eta_G(T) < 2$, and has finite cusp singularities when $\eta_G(T) > 2$. In principle, this can be seen by X-ray or neutron diffraction, and the exponent $\eta_G(T)$ measured, which would be a rigorous experimental test of the theory. Unfortunately, this has not been possible because the required resolution in $\mathbf{q}$ has not been achieved to date.

Earlier, we argued that, if the 2D crystal contains a finite concentration of free, unbound dislocations, then, under an arbitrarily small shear stress, these dislocations move to relax the stress to zero, so that the crystal has a fluid-like response to the stress. Thus, the system with free dislocations is melted and is a fluid at long length scales. Also, we were certain that the full dislocation Hamiltonian of Eq. (1.93) would yield the detailed behavior of the 2D system at the melting transition. However, around 1973, there was some controversy about the relative sign of the two terms in the dislocation part, $H_D$, of the Hamiltonian of Eq. (1.93). At the time, this apparently minor technical problem seemed unimportant, because the vital term seems to be the $\ln r$ term in the interaction, as this dominates the
angular term at large separations $r$. Ignoring the angular term leads to a rather uninteresting (and incorrect) problem so, fortunately, we did no more with it. A few years later, Halperin, Nelson and Young solved the melting problem properly\textsuperscript{42,43} by treating the angular term in $H_D$ correctly. The hexatic phase was discovered and the modern KTHNY theory of melting was born.

The natural way to go beyond the Gaussian theory, which uses only the smooth part of the lattice displacements in $H_0$ of Eq. (1.93), is to compute perturbative corrections to the bare elastic moduli due to dislocations as a power series in the dislocation fugacity $y = \exp(-E_c/k_BT)$. This can be done in an analogous way to computing the renormalized stiffness $\rho^s_R$ of Sec. 1.5 for a superfluid film. One must first identify the appropriate correlation function from which the renormalized elastic constants $\mu_R(T)$ and $\lambda_R(T)$ can be extracted. This has been done by Halperin and Nelson\textsuperscript{42} by expressing the tensor of renormalized elastic constants in terms of a correlation function,

\begin{equation}
C_{ijkl} = \tilde{\mu}_R(T)(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \tilde{\lambda}_R(T)\delta_{ij}\delta_{kl},
\end{equation}

where $\Omega$ is the area of the crystal, $\mathbf{n}$ is a unit vector normal to the edge of the system directed outwards, and the integration is over the perimeter $P$ of the crystal. Remembering that, in the presence of dislocations, the displacement field, $u(r)$, is multivalued,\textsuperscript{77} one can apply Green’s theorem to $U_{ij}$ in Eq. (1.95) to obtain

\begin{equation}
U_{ij} = -\frac{1}{2} \oint_P dl(u_in_j + u_jn_i),
\end{equation}

Now that we have identified the appropriate correlation function defining the renormalized elastic moduli, $\tilde{\mu}_R$ and $\tilde{\lambda}_R$, all that remains is some tedious but straightforward algebra to obtain the recursion relations for the running coupling constants under a rescaling of the short distance cut off, $a \to ae^\delta_l$.\textsuperscript{42}
Early Work on Defect Driven Phase Transitions

\[ \frac{d \mu^{-1}(l)}{dl} = 3\pi y^2(l)e^{K(l)/8\pi} I_0\left(\frac{K(l)}{8\pi}\right) + O(y^3), \]

\[ \frac{d(\tilde{\mu}(l) + \tilde{\lambda}(l))^{-1}}{dl} = 3\pi y^2(l)e^{K(l)/8\pi} \left[ I_0\left(\frac{K(l)}{8\pi}\right) - I_1\left(\frac{K(l)}{8\pi}\right) \right] + O(y^3), \]

\[ \frac{dy(l)}{dl} = \left(2 - \frac{K(l)}{8\pi}\right)y(l) + 2\pi y^2(l)e^{K(l)/16\pi} I_0\left(\frac{K(l)}{8\pi}\right) + O(y^3), \]

\[ \frac{dK^{-1}(l)}{dl} = \frac{4\tilde{\mu}(l)(\tilde{\mu}(l) + \tilde{\lambda}(l))}{2\tilde{\mu}(l) + \tilde{\lambda}(l)}, \]

(1.97)

where \( I_0(x) \) and \( I_1(x) \) are modified Bessel functions.

The recursion relations of Eq. (1.97) have flows for the parameters, \( \tilde{\mu}(l) \), \( \tilde{\lambda}(l) \), and \( y(l) \), very similar to Eq. (1.35) for the XY model. Above a temperature, \( T_m \), the dislocation fugacity, \( y(l) \), increases as \( l \) increases, implying that dislocations unbind and become free to move under any small stress, so that the crystal has melted. We can integrate these flow equations up to a length scale \( \xi_+(T) \), where

\[ \xi_+(T) = e^{\nu} = \exp(b't^{-\nu}) \quad \text{with} \quad \nu = 0.3696 \cdots. \]

(1.98)

The scale \( \xi_+(T) \) is interpreted as the scale below which dislocations can be regarded as bound in pairs or triplets, while, on scales larger than \( \xi_+(T) \), dislocations must be regarded as free to move under arbitrarily small stress, so that the system responds like a fluid and has melted. On the other hand, for \( T \leq T_m \), the fugacity, \( y(l) \), flows to the stable Gaussian fixed line \( y(\infty) = 0 \), and the renormalized elastic constants \( \tilde{\mu}_R(T) \) and \( \tilde{\lambda}_R(T) \) have finite values, in the same way as the renormalized superfluid density \( \rho_0^R(T) \).

Thus, the low temperature phase of this system is an elastic solid with finite elastic constants, neither of which are universal at \( T_m^- \). For \( T \leq T_m \), from Eq. (1.97), one obtains

\[ \tilde{\mu}_R(T) = \tilde{\mu}_R(T_m^-)(1 + b|t|^{\nu'}), \]

(1.99)

\[ \tilde{\lambda}_R(T) = \tilde{\lambda}_R(T_m^-)(1 + b|t|^{\nu'}). \]

Although these elastic moduli are not individually universal at \( T = T_m^- \), the
combination $K_R(T_m)$ is universal. From Eq. (1.97), we have

$$K_R(T_m) = \frac{4\tilde{\mu}_R(\tilde{\mu}_R + \tilde{\lambda}_R)}{2\tilde{\mu}_R + \tilde{\lambda}_R} = \lim_{l \to \infty} K(l) = 16\pi. \quad (1.100)$$

The flow equations of Eq. (1.97) are very similar to Eq. (1.35) for the planar rotor model and the solutions also behave similarly. There is one major complication in the dislocation case for a solid with an underlying triangular symmetry. A bound pair of elementary dislocations can be equivalent to a third elementary dislocation, which leads to the $O(y^2)$ contribution to the fugacity, $y(l)$, flow in Eq. (1.97). Although this does not make a major qualitative difference from the planar rotor vortex behavior, it does introduce some major technical complications, and gives a value of the exponent $\nu = \frac{3696}{3696} \cdot \cdots$ which is different from the planar rotor value of $\nu = \frac{1}{2}$. At present, this difference in $\nu$ from $1/2$ is beyond experimental resolution.

One can also obtain the measured or renormalized Debye–Waller factor, which is closely related to the pair distribution function,

$$g(r) = \frac{\Omega}{N^2} \left( \sum_{ij} \delta(r - r_i + r_j) \right), \quad (1.101)$$

and the Debye–Waller factor is

$$C_G(r) = \langle \rho_G(r)\rho_G(0) \rangle \sim r^{-\eta_G(T)},$$

$$\eta_G(T) = \frac{|G|^2}{4\pi} \frac{3\tilde{\mu}_R + \tilde{\lambda}_R}{\tilde{\mu}_R(2\tilde{\mu}_R + \tilde{\lambda}_R)}. \quad (1.102)$$

Here, the $T$ dependence has been absorbed into the renormalized elastic moduli, $\tilde{\mu}_R(T)$ and $\tilde{\lambda}_R(T)$, of Eq. (1.99). The numerical value of $\eta_G(T)$ cannot be calculated exactly because the elastic moduli $\tilde{\mu}_R(T)$ and $\tilde{\lambda}_R(T)$ are not individually universal. However, for long ranged repulsive interactions, it is clear that $\tilde{\lambda}_R \gg \tilde{\mu}_R$ so that $\eta_G(T) \approx |G|^2/(4\pi\tilde{\mu}_R(T))$. The smallest value of $\eta_G$ gives the dominant behavior of $C_G(r)$ and, for a hexagonal crystal, $\eta_G(T_m) \geq \eta_G_0(T_m) = 1/3$.

At $T > T_m$, the dislocation fugacity is relevant, which implies that there is a finite density of free dislocations in the system. These can be regarded as bound in pairs up to a length scale $e^{l^*} = \xi_+(T)$ of Eq. (1.98), but are free, unbound at larger scales. The positional correlation function is expected to decay exponentially as

$$C_G(r) \sim e^{-r/\xi_+(T)} \quad \text{for} \quad r \gg \xi_+(T). \quad (1.103)$$

Also, when $T > T_m$, the length dependent elastic moduli $\mu_R(l), \lambda_R(l) = 0$ for $e^l > \xi_+(T)$ but will be finite at length scales $e^l < \xi_+(T)$. This is an example
of a system which has solid-like behavior at short length scales, \( e^l < \xi_+(T) \) and is fluid-like at larger scales. This behavior is analogous to the behavior of the scale dependent stiffness constant \( K(l) \) of the planar rotor model of Sec. 1.5.

We now discuss the behavior of the fluid phase when all dislocation pairs and triplets are unbound. This fluid phase is not the familiar isotropic fluid, but has remnants of the six-fold orientational order of the underlying triangular lattice of the low temperature solid phase. These possible orientational correlations in the fluid can be characterized by a finite renormalized Frank constant \( K_A(T) \) of the anisotropic fluid. This can be expressed as a bond angle correlation function,

\[
K_A^{-1}(T) = \lim_{q \to 0} \frac{q^2}{\Omega} \langle \theta(q)\theta(-q) \rangle. \tag{1.104}
\]

The orientational correlations in a fluid are characterized by \( \infty > K_A^{-1}(T) > 0 \), so a finite value of \( K_A(T) \) implies that the fluid has orientational correlations. At temperatures, \( T > T_m \), we expect exponential decay of translational order as \( \exp(-r/\xi_+(T)) \), but the system is elastic up to a length scale \( e^l = \xi_+(T) \), and the dislocations are free at larger scales. One expects that the bond angles to be controlled by a free energy,

\[
\frac{F_A}{k_B T} = \frac{1}{2} K_A \int d^2 r (\nabla \theta)^2. \tag{1.105}
\]

In the solid, the bond angle, \( \theta_s(r) \), due to a set of dislocations is

\[
\theta_s(r) = -\frac{a_0}{2\pi} \sum_{r'} \frac{\mathbf{b}(r') \cdot (r - r')}{|r - r'|^2}, \tag{1.106}
\]

from which one can express the stiffness constant as a correlation function,

\[
K_A^{-1} = \lim_{q \to 0} \frac{a_0^2 q_i q_j}{\Omega q^2} \langle b_i(q)b_j(-q) \rangle. \tag{1.107}
\]

The dislocation correlation function is calculated from the dislocation free energy of Eq. (1.93), written in Fourier space as,

\[
\frac{H_D}{k_B T} = \frac{1}{2\Omega} \sum_q \left( \frac{K}{q^2} \left[ \delta_{ij} - \frac{q_i q_j}{q^2} \right] + \frac{2E_c a^2}{k_B T} \delta_{ij} \right) b_i(q)b_j(-q). \tag{1.108}
\]

At this point, we can see why the sign of the angular term in the dislocation interaction is vital and, also, why ignoring the angular term leads to incorrect results. The existence of a finite Frank constant, \( K_A(T) \), depends on the transverse projection operator in the dislocation energy of Eq. (1.108), which arises from the form of the dislocation interaction of Eq. (1.93).
To proceed, we use the recursion relations of Eq. (1.97) up to some \( l \leq \ell^* = \ln \xi_+ (T) \), when they are still valid, to obtain,

\[
K_A (T) = K_A (\tilde{\mu}, \tilde{\lambda}, y) = e^{2l} K_A (\tilde{\mu} (l), \tilde{\lambda} (l), y (l)),
\]

(1.109)
since there are two additional factors of \( q \) in the definition of \( K_A \) compared to \( \tilde{\mu}, \tilde{\lambda} \). At the scale \( e^{l^*} = \xi_+ (T) \), we can assume that the density of free dislocations is large, and a reasonable approximation is to regard the field \( b(q) \) as continuous, ignoring the discrete nature of the \( b(r) \). This Debye–Hückel approximation allows the correlation function in Eq. (1.107) to be computed, because the transverse part in \( H_D \) of Eq. (1.108) does not contribute. We obtain,

\[
K_A^{-1} (T) \approx \frac{k_B T}{2E_c a^2} > 0,
\]

(1.110)

which establishes that the fluid has orientational correlations.

We are left with a 2D XY problem with initial parameter \( K_A (l^*) \), which we know how to solve. The topological defects which control the six-fold orientational order, when \( T > T_m \), are \( \pm \pi / 3 \) disclinations in the underlying hexagonal lattice. These are precisely analogous to the vortices in a 2D superfluid, and we can decompose the bond angle field \( \theta(r) \) into a smooth part \( \phi(r) \) and a singular part due to a set of disclinations to obtain,

\[
\frac{H_D}{k_B T} = \frac{1}{2} \int d^2 r (\nabla \phi (r))^2 - \frac{\pi K_A}{36} \sum_{r \neq r'} m(r) m(r') \ln \left( \frac{|r - r'|}{a} \right) + \frac{E_c}{k_B T} \sum_r m^2 (r). \tag{1.111}
\]

Here, \( m(r) = 0, \pm 1, \pm 2 \cdots \) is an integer measure of the strength of the disclination at \( r \), \( a \) is the disclination core size, \( E_c \) the disclination core energy, and the disclinations are subject to the neutrality condition, \( \sum_r m(r) = 0 \). We can immediately take over the results for the 2D superfluid of Sec. 1.5 to deduce that a disclination unbinding transition occurs at \( T = T_I \), when

\[
\frac{36}{2\pi K_A (T_m)} = \frac{1}{4}. \tag{1.112}
\]

The renormalized Frank constant, \( K_A (T) \), behaves just like the stiffness constant, \( K_R (T) \), of the 2D superfluid, and jumps discontinuously to zero at \( T_I \),

\[
K_A (T) = \frac{72}{\pi} (1 + b|t|^{1/2}), \quad \text{when } t = \frac{(T - T_I)}{T_I} \leq 0,
\]

\[
K_A (T) = 0, \quad \text{when } t > 0. \tag{1.113}
\]
When $T > T_I$, the orientational order is short ranged with
\[ \langle \psi_6(r)\psi_6^*(0) \rangle \sim e^{-r/\xi_6(T)}, \tag{1.114} \]
where the orientational correlation length, $\xi_6(T)$, diverges exponentially,
\[ \xi_6(T) = \exp\left(\frac{b}{(T/T_I - 1)^{1/2}}\right). \tag{1.115} \]

Assuming the initial value of $K_A(l)$ is larger than the critical value, it will flow to a value $K_A(\infty) \geq 72/\pi$. For $T$ just above the melting temperature, $T_m$, we expect that $K_A(T) \sim \xi_2^2(T)$, and, at the hexatic-isotropic liquid transition temperature, $T_I$, this theory predicts that $K_A(T_I) = 72/\pi$. Presumably, if the core energy $E_c$ is, for some reason, small so that the initial $K_A(l^*) < K_{0c}$, it will immediately flow to zero and there will be no hexatic phase. It is also possible that the hexatic phase exists over a very narrow temperature interval, $T_m < T \leq T_I$. Below the melting temperature, in the crystal phase, the correlation length $\xi_2(T) = \infty$, so that $K_A(T \leq T_m) = \infty$, and there is true long range orientational order. Alternatively, one can calculate $\langle \psi(r)\psi^*(0) \rangle$ at $r = \infty$ and find that it is finite,$^{42}$
\[ \langle |\langle \psi(r)\rangle| \rangle \approx \exp\left(-\frac{9k_BT}{8\pi\mu R(T)}\right) > 0. \tag{1.116} \]
This was noticed earlier by Mermin.$^{56}$

1.6.4. **Substrate effects on 2D melting**

Most experiments on 2D melting are performed on a layer of adsorbed molecules on some substrate such as graphite, which forms relatively large well oriented domains of a periodic array of binding sites. It is therefore important to assess the effects of such a substrate. In their seminal paper,$^{42}$ Halperin and Nelson performed this investigation, summarized below. Both the graphite substrate and the adsorbate overlayer have the same six-fold orientational symmetry, allowing the relative orientations to vary slowly in space leading to an elastic free energy,
\[ \frac{H}{k_BT} = -\frac{1}{2k_BT} \int \frac{d^2q}{(2\pi)^2} u_i(q)D_{ij}(q)u_j(-q) + \sum_{r,K} h_K e^{iK \cdot r} (1 + iK \cdot u(r) + \cdots) \tag{1.117} \]
\[ D_{ij}(q) = \mu_R q^2 \delta_{ij} + (\mu_L + \lambda_R)q_i q_j. \]
Here, one has assumed that the substrate potential can be written as \( \sum_K h_K e^{iK \cdot r + u(r)} \), where \( \{K\} \) are the reciprocal lattice vectors of the periodic substrate potential. These are incommensurate with the reciprocal lattice vectors \( \{G\} \) of the overlayer. Another assumption is that the adsorbate is in its low temperature floating solid phase, described by a harmonic free energy with renormalized elastic constants \( \mu_R \) and \( \lambda_R \). By redefining the displacement field,

\[
u_i(q) \to u_i'(q) = u_i(q) + iD_{ij}^{-1}(q) \sum_K h_K K_j \Delta_{K,q}
\]

\[
\Delta_{K,q} = 1 \text{ if } K = q + G
\]

\[
\frac{H}{k_B T} = \frac{1}{2k_B T} \int \frac{d^2 q}{(2\pi)^2} u_i'(q)D_{ij}(q)u_j'(-q) - \frac{\Omega}{2} \sum_K h_K^2 K_i D_{ij}^{-1}(K) K_j
\]

where \( \{G\} \) is a reciprocal lattice vector of the adsorbed layer. One can write the second term in Eq. (1.118) as

\[
C(\theta) = -\frac{\Omega}{2} \sum_K \sum_{s=1}^2 h_K^2 \left( \frac{K \cdot \hat{\epsilon}_s(K)}{\omega_s(K)} \right)^2,
\]

(1.119)

where \( \hat{\epsilon}_s(K) \) is the \( s \)th polarization vector and \( \omega_s(K) \) is the eigenfrequency of the matrix \( D_{ij}(K) \).

Now, for a triangular adsorbate on a triangular substrate, \( \theta = 0 \) means perfect alignment, and the Fourier series is

\[
C(\theta) = \Omega \sum_{k=0}^{\infty} c_k \cos(6k\theta)
\]

(1.120)

and, for a triangular adsorbate on a square substrate,

\[
C(\theta) = \Omega \sum_{k=0}^{\infty} c_k \cos(12k\theta).
\]

(1.121)

Note that we have assumed that the adsorbate has a periodicity \( G \) which is incommensurate with the substrate periodicity \( K \), so that the only effect of the substrate potential is on the orientation of the crystal axes of the adsorbate. One can investigate the dislocation induced melting of the incommensurate adsorbate by writing the displacement as \( u = \phi + u_s \), where \( u_s \) is the part due to the dislocations.
After some straightforward but tedious algebra, one finds that the elastic free energy can be written as,

\[
\frac{H_{E}}{k_{B}T} = \frac{1}{2} \int \frac{d^{2}r}{a_{0}^{2}} (2\tilde{\mu}\phi_{ij}^{2} + \tilde{\lambda}\phi_{kk}^{2} + \tilde{\gamma}(\partial_{y}\phi_{x} - \partial_{x}\phi_{y})^{2}) + \frac{H_{D}}{k_{B}T},
\]

\[
\frac{H_{D}}{k_{B}T} = -\frac{1}{8\pi} \sum_{r \neq r'} b_{i}(r)b_{j}(r') \left( K_{1} \ln \frac{|r - r'|}{a} \delta_{ij} - K_{2} \frac{(r - r')(r - r')}{|r - r'|^{2}} \right) + \frac{E_{c}}{k_{B}T} \sum_{r} |b(r)|^{2},
\]

(1.122)

\[
K_{1} = \frac{4\tilde{\mu}(\tilde{\mu} + \tilde{\lambda})}{2\tilde{\mu} + \tilde{\lambda}} + \frac{4\tilde{\mu}\tilde{\gamma}}{\tilde{\mu} + \tilde{\gamma}},
\]

\[
K_{2} = \frac{4\tilde{\mu}(\tilde{\mu} + \tilde{\lambda})}{2\tilde{\mu} + \tilde{\lambda}} - \frac{4\tilde{\mu}\tilde{\gamma}}{\tilde{\mu} + \tilde{\gamma}}.
\]

The renormalization group flows for the parameters \(K_{1}(l)\), \(K_{2}(l)\) and \(y(l)\) were first worked out by Young\(^{43}\) who showed that

\[
\frac{dy}{dl} = \left( 2 - \frac{K_{1}}{8\pi} \right) y + 2\pi y^{2} I_{0} \left( \frac{K_{2}}{8\pi} \right) + O(y^{3}).
\]

(1.123)

The same physics as for the isotropic elastic solid, when \(K_{2} = K_{1}\), holds in the ordered phase. Melting happens at \(K_{1R}(T_{m}^{-}) = 16\pi\) and \(K_{2R}(T_{m}^{-})\) has some finite value depending on the orientational coupling strength, \(\gamma_{R}(T_{m}^{-})\).

The relative values of the \(K_{i}\) depend on the lattice structures of the substrate and the overlayer. The value of the exponent \(\nu\) in Eqs. (1.98) and (1.99) depend on the value of \(K_{2R}\).\(^{42,43}\)

In the situation, when the substrate and overlayer reciprocal lattice vectors, \(\{K\}\), \(\{G\}\), have a set, \(\{M\}\), in common, there is the possibility that the overlayer is locked to the substrate, and so is a commensurate locked phase. We consider the smallest common vectors of length \(M_{0} = |M|\) and write the Hamiltonian as,\(^{42}\)

\[
\frac{H}{k_{B}T} = \frac{H_{E}}{k_{B}T} + \sum_{|M|=M_{0}} h_{M} \sum_{R} e^{iM \cdot u(R)},
\]

(1.124)
where we assume that the effects of all other incommensurate terms have been incorporated into the elastic Hamiltonian, $H_E$. This is possible because these and commensurate terms in the substrate potential, $H_s$

$$h_K = \sum_K \sum_r e^{iK \cdot u(r)}, \quad (1.125)$$

with $|M| > M_0$ are less relevant than $|M| = M_0$.

To assess the relevance of $h_M$, we calculate the correlation function with a renormalized elastic Hamiltonian, $H_E$, with $h_M = 0$,

$$\langle e^{iM \cdot [u(r) - u(0)]} \rangle_{H_E} \sim r^{-\eta_M}, \quad (1.126)$$

$$\eta_M(T) = \frac{M_0^2 k_B T}{4\pi} \frac{3\mu_R + \lambda_R + \gamma_R}{(\mu_R + \gamma_R)(2\mu_R + \lambda_R)}. \quad (1.127)$$

From this, we can see immediately that the RG eigenvalue associated with $h_{M_0}(l) = h_{M_0}(0)e^{\lambda_{M_0} l}$ is

$$\lambda_{M_0}(T) = 2 - \frac{1}{2}\eta_{M_0}$$

$$= 2 - \frac{M_0^2 k_B T}{8\pi} \frac{3\mu_R + \lambda_R + \gamma_R}{(\mu_R + \gamma_R)(2\mu_R + \lambda_R)}. \quad (1.127)$$

From Eq. (1.127), we see that, at low enough $T$, all the $h_M$ are relevant, and the overlayer is locked to the substrate, implying that a lattice gas description is appropriate. The substrate mesh is sufficiently coarse, $\lambda_{M_0}(T_m) > 0$, which means that the overlayer is locked to the substrate up to the melting temperature, $T_m$, for $h_M = 0$. The dislocation melting mechanism is not appropriate at any $T$ in this case. For large $M_0$, corresponding to a finer substrate mesh, $\lambda_{M_0}(T_m) < 0$, the overlayer will become unlocked from the substrate at some $T < T_m$, leading to a floating incommensurate solid, which may be accidentally commensurate with the substrate. One can also derive a criterion for the temperature, $T < T_m$, at which the overlayer unlocks from the substrate.\(^{32}\)

The most dramatic effect of the substrate potential, even when it does not lock the overlayer into a commensurate phase, is on the fluid phases for $T > T_m$. We can perform a similar analysis for the Frank constant $K_A$ defined as a correlation function in Eq. (1.107), using a Debye–Hückel approximation with the dislocation Hamiltonian, $H_D$, of Eq. (1.122). Since, as in Eq. (1.107), to compute $K_A$, we require the correlation function, in the
Debye–Hückel approximation,
\[ K_A^{-1} = \lim_{q \to 0} \frac{\alpha_0^2 \Omega^2}{q^2} \langle b_i(q)b_j(-q) \rangle, \]
\[ \langle b_i(q)b_j(-q) \rangle = \frac{2\Omega q^2}{K_1 + K_2 + \frac{4E_c a^2}{k_B T}} \left( \delta_{ij} - \frac{q_i q_j}{q^2} \right) + \frac{2\Omega q^2}{K_1 - K_2 + \frac{4E_c a^2}{k_B T}} \frac{q_i q_j}{q^2}, \]
\[ K_A^{-1}(T) = \lim_{q \to 0} \frac{2q^2}{K_1 - K_2 + \frac{4E_c a^2}{k_B T}} = 0, \text{ for } K_1 \neq K_2. \]

Thus, we recover the smooth substrate result that \( K_A > 0 \), while, for melting on a periodic substrate, \( K_A(T) = \infty \). This means that there is no hexatic-isotropic fluid transition on any periodic triangular substrate, as the orientation of the hexatic fluid remains locked to the substrate orientation at all \( T > T_m \). For a triangular adsorbate on a substrate with a weak binding potential of square symmetry, the hexatic-isotropic transition will be in the 2D Ising universality class.

### 1.6.5. Scaling in superconducting films

We can write a scaling assumption for the resistivity \( R \), consistent with the renormalization group, by introducing all the relevant length scales, \( \lambda_{\text{eff}}, \xi_+, \xi_-, \), and \( \xi_I \). The scales \( \xi_+ = \xi_+^{2n} \) of Eq. (1.45) depend on \( T \) only, while \( \xi_I = I/I_0 \) is the current length scale, and the penetration depth \( \lambda_{\text{eff}} \) is an effective system size. We can make the scaling ansatz,\(^{117}\)
\[ \frac{V}{T} = e^{-z l \xi_+^{2n}} R(\lambda_{\text{eff}} e^{-1}, \xi_+ e^{-1}, \xi_I e^{-1}, l/\ln \xi_+), \] (1.129)

where the dynamical exponent \( z = 2 \), and \( R \) is an unknown scaling function, familiar from more conventional scaling functions, except for the combination \( l/\ln \xi_- \), which arises from the marginally relevant and irrelevant scaling fields of the problem. The effect of this combination is to produce temperature and current dependent power laws, after making an appropriate choice for the length scale \( e^l \) such that the scaling function \( R \) is known or can be computed. In this system, there are four potentially divergent length scales, \( \xi_+, \xi_-, \xi_I, \lambda_{\text{eff}} \), and \( \xi_{\text{eff}} \), so the behavior of the scaling function and the IV characteristics are very complex and difficult to obtain.

However, when the current \( I \) is not too small so that \( \xi_I < \xi_+, \lambda_{\text{eff}} \), one can choose the arbitrary scale \( e^l = \xi_I \). At this scale, all vortex pairs are
unbound by the current, and the free vortices may be regarded as moving independently, driven by the current in a viscous medium, so that

\[ V/I = I^2 R(\lambda_{\text{eff}}/\xi_1, \xi_+/\xi_1, 1, \ln \xi_I/\ln \xi_-). \]  \hfill (1.130)

For \( T \leq T_{KT} \) and \( \lambda_{\text{eff}} > \xi_I > \xi_- \), we expect that

\[ R(\infty, \infty, \ln \xi_I/\ln \xi_-) \sim I^{1/\ln \xi_-(T)} \sim I^{2(T)}, \]  \hfill (1.131)

where \( \xi_-(T) = \exp[1/x(T)] \) with \( x(T) = b[T - T_{KT}]^{1/2} \), which leads to the usual nonlinear IV relation \( V \sim I^\pi K_R(T) + 1 \). \cite{55a} When \( \ln \xi_I < \ln \xi_- \), we expect that \( V \sim I^3 \) which is the IV characteristic at \( T_{KT} \) when \( \xi_-(T) \to \infty \). Finite size dominated behavior is also contained in Eq. (1.129) by taking \( \lambda_{\text{eff}} < \xi_I \) and \( e^I = \lambda_{\text{eff}} \) to obtain

\[ V/I = \lambda_{\text{eff}}^{-2} R(1, \infty, \xi_I/\lambda_{\text{eff}}, \ln \xi_I/\ln \xi_-) \sim \lambda_{\text{eff}}^{-2}. \]  \hfill (1.132)

Identical arguments lead to a linear IV relation \( V/I \sim \lambda_{\text{eff}}^{-\pi K_R(T)} \) when \( \lambda_{\text{eff}} > \xi_- \) and \( V/I \sim \lambda_{\text{eff}}^{-2} \) when \( \lambda_{\text{eff}} < \xi_- \). In principle, in the scaling regime of large correlation lengths one should be able to obtain analytically the scaling function \( R \), but this has not yet been achieved. Some simulations have been performed on lattice models of coupled Josephson junctions in a square array \cite{117} which agree with the analytic predictions of Refs. 67 and 55, while other simulations \cite{116} disagree obtaining \( V \sim I^{2\pi K_R(T)-1} \), which agrees with the AHNS theory \cite{67} only at \( T = T_{KT} \), but not for any other temperature.

Experimental measurements of the IV relation are, in general, consistent with the power law relation \( V \sim I^a(T) \), with \( a(T) = \pi K_R(T) + 1 \) at intermediate values of the current \( I \), but there is no discontinuity of the power \( a(T) \) where \( a(T) \geq 3 \) for \( T \leq T_{KT} \) and \( a(T) = 1 \) for \( T > T_{KT} \).\cite{118}

Some measurements find evidence for a KT transition as these use a system with a very large penetration depth.\cite{119,120,121} However, theory\cite{17} predicts that there should be no true superconducting phase at any \( T > 0 \) because there would always be a finite concentration of free unbound vortices \( n_f \) and \( V/I \sim n_f > 0 \) for sufficiently small \( I \). In dirty superconducting films, the penetration depth \( \lambda_{\text{eff}} \) is sufficiently large so that \( n_f \ll 1 \) and the linear resistivity is swamped by finite current effects. However, measurements on small arrays of Josephson junctions,\cite{122} and on films of YBCO one unit cell thick,\cite{123} find indications of a linear IV relation at very small currents at low \( T < T_{KT} \), indicating a finite concentration of free vortices and no KT transition, as predicted in an early paper.\cite{17} The conclusion one seems to be forced to adopt is that, in superconducting films, the \( I \to 0 \) predictions are
not accessible because of finite current effects, and a full crossover analysis is needed to fit the experimental data.

1.7. Experiments and Simulation

We have already given, in Sec. 1.5, a brief discussion of the key experiments\textsuperscript{21,66,69} that have established the linear relation between the minimum superfluid density at which superfluidity can exist and the transition temperature at which this occurs. In this section we give a fuller discussion of these experiments. We also discuss experiments on other systems which can have transitions controlled by defects, and simulations of such systems, both simulations based on computer calculations, and those based on fabricated analog systems.

1.7.1. Measurements on superfluid films

The first thing to notice is that the superfluid density is, in fact, the $q, \omega \to 0$ limit of a response function. The Bishop–Reppy torsional oscillator experiment\textsuperscript{66} measures the resonant frequency and the drive needed to overcome the damping due both to the torsion fiber and, in the neighborhood of the transition temperature, to the mutual friction between the normal fluid and the superfluid, the complex frequency dependent behavior of $\rho_s^R(q = 0, \omega)$ where $\omega$ is the oscillation frequency of the torsional oscillator. The force exerted by the film on the oscillating substrate leads to a shift $\Delta P$ in the period $P$ of the oscillator, and the power dissipated in the film leads to a finite $Q$ factor\textsuperscript{67} where

$$\frac{\Delta P}{P} = \frac{A}{2M} \text{Re}[\rho_s^R(\omega)],$$

$$Q^{-1} = -\frac{A}{M} \text{Im}[\rho_s^R(\omega)].$$

(1.133)

Here, $A$ is the area of the substrate, $M$ is the mass of the oscillating substrate and $\omega$ is the frequency of oscillation. The extension of the Kosterlitz–Thouless static theory to finite frequency was essential for the comparison to experiment because, by necessity, the superfluid density is measured in a dynamical experiment at finite $\omega$ and finite superfluid velocity $u_s$. The conventional interpretation of the superfluid density is at $u_s = \omega = q = 0$ which is not accessible to experiment. The BKT static theory predicts only the $\omega = q = 0$ component of $\rho_s^R(q, \omega)$. The AHNS theory\textsuperscript{67} for $\rho_s^R(q, \omega, v_n)$ is based on the static theory and yields an excellent fit to the torsional oscillator experiments and to third sound measurements\textsuperscript{69,70} which also indicated that
$\rho_s^R(T_c^-) > 0$. This is in contrast to superfluids in 3D where the superfluid density vanishes at $T_c$.

In the torsional oscillator experiments at higher temperatures, where the helium is a normal liquid, the fluid moves with the substrate, and so the position of the resonance is determined in the usual way by the stiffness of the torsion thread, and by the total classical moment of inertia of the combination of the Mylar roll and the liquid film adhering to it. Most of the damping of the oscillator comes from dissipative effects in the torsion thread, with some small contribution from the viscosity of the helium gas surrounding the rotating cylinder. As the transition temperature is approached from above there begin to be regions which are superfluid, presumably predominantly in regions where the helium film is thickest, and such superfluid regions need to move with potential flow, $\nabla \times \mathbf{v} = 0$. Such regions of superfluidity reduce the moment of inertia of the film and increase the damping of the oscillator, so the onset of superfluidity is marked by an increase in the frequency of the torsional oscillator and a reduction in its amplitude. As the temperature is lowered further, the whole film becomes superfluid, with a superfluid density that tends to a limit lower than the total density of the film (in particular, the layer in contact with the solid never shares in the superfluidity), while the damping has a sharp maximum close to the superfluid transition, and is significant, but well below the maximum.

In the paper by Bishop and Reppy, a figure to display the linear relation between transition temperature and the superfluid density (per unit area) at the transition is combined with experimental results based on measurements of third sound speed and attenuation. Third sound is a surface wave in a superfluid, which involves a wave in the superfluid density, balanced by a wave motion of the entropy, so that the normal fluid atoms, locked to the substrate, do not have to move. The analysis of this system is more complicated than the analysis of the torsion oscillator. We have already mentioned that Rudnick’s group published an analysis showing a discontinuity of $\rho_s$ in 1969, but published a reanalysis a year later which no longer claimed this discontinuity of the superfluid density at the phase transition.

1.7.2. **Experimental measurements on 2D melting**

Around 1980, all these interesting theoretical predictions for a solid/hexatic/fluid system in 2D were known, in particular that a 2D crystal melts, at temperature $T_m$, to an anisotropic hexatic fluid by a continuous transition. At temperature $T_I > T_m$, the hexatic fluid transitions to an
isotropic fluid via another continuous transition. This is in contrast to measurements of melting in 3D, which seems always to be a discontinuous first order transition. Also, prior to this, melting in 2D was believed by almost all physicists to be a single first order transition directly to an isotropic fluid. The status of the 2D melting problem in 1988 is reviewed in depth by Strandburg. The status of 2D solids and fluids was already under fairly intense scrutiny, but with little success, although apparently continuous melting transitions were observed in several systems, and a continuous hexatic to isotropic fluid transition in a few cases. The natural sequence of experimental studies of melting in 2D would be to study first the simplest system of particles confined to a plane by a smooth, featureless potential to eliminate any extra complications. Unfortunately, this simplicity was not realized experimentally until 1999.

The experimental challenge is to find convincing evidence for or against the appealing theoretical picture of a two-stage melting process, with an intervening anisotropic hexatic fluid phase between the low temperature triangular crystal phase and the high temperature isotropic fluid. An experiment to test the dislocation theory of melting must satisfy at least two conflicting criteria, a large, flat, well characterized substrate to support the system, and, preferably, featureless to avoid as many complications as possible. Ideally, a solid state substrate should be atomically flat, with no steps, over distances of several correlation lengths, $\xi(T)$, which diverge exponentially near the transitions. A typical domain on a flat substrate is less than $10^4$ atomic spacings, which can be exceeded by $\xi(T)$, implying that measurements tend to be finite size limited. Another major problem with solid state substrates is that they tend to be a crystal surface. Graphite cleaves into fairly large, atomically flat regions, which seem ideal until one remembers that a graphite surface tends to be a set of binding sites which form a triangular lattice of a certain spacing which may not be commensurate with the natural spacing of the adsorbate lattice. The most obvious effect of a graphite substrate is to impose a hexatic ordering field which induces long range hexatic order in the adsorbed layer, so that the fluid phase is a hexatic fluid at all $T > T_m$. Experiments on xenon adsorbed on graphite, and on the (111) face of silver are consistent with this. An extensive survey of experiments with different combinations of adsorbates and substrates is in Strandburg’s review article. As shown in Sec. 1.6.4, the solid still melts due to dislocations and the transition is characterized by slightly different singularities than melting on a smooth substrate, but the differences are beyond present experimental resolution.
The first attempt to investigate the melting of a $2D$ periodic crystal, without the extra complications of a periodic substrate, was done by Grimes and Adams.\textsuperscript{101} They trapped a layer of electrons of density, $n_s = 10^8 - 10^9 \text{cm}^{-2}$, approximately 100 Å above the surface of superfluid $^4\text{He}$. In this range of density, the electrons behave classically, with a repulsive $1/r$ Coulomb interaction, characterized by a dimensionless parameter, $\Gamma = e^2 \sqrt{\pi n_s} / k_B T$, where $n_s$ is the number density. For $\Gamma > \Gamma_c = 137 \pm 15$, the electrons form a hexagonal lattice, whose longitudinal vibrations are coupled to surface waves of the $^4\text{He}$.\textsuperscript{102} This coupled system has measurable response functions, which allow one to draw some conclusions about the electron lattice. There is no discontinuity in the frequency or amplitude of the resonances as $\Gamma$ is varied, but there is a pronounced maximum in the amplitude at $\Gamma \approx 137$, and no hysteresis in the response. From this, one can conclude that the lattice melts at $\Gamma = \Gamma_m = 137 \pm 15$ by a continuous transition, consistent with KTHNY theory.\textsuperscript{102} Thouless attempted to calculate $\Gamma_m$\textsuperscript{103} using the $T = 0$ values, $\lambda = \infty$ and $\mu = 0.245 e^2 n^{3/2}$, in $k_B T_m = a_0^2 \mu$ to obtain $\Gamma_m = (\pi n)^{1/2} e^2 / (k_B T_m) = 78.71$, which differs from the experimental value of $\Gamma_m = 137 \pm 15$.\textsuperscript{101} A value $\Gamma_m \approx 95 \pm 2$ was obtained by Hockney and Brown using molecular dynamics.\textsuperscript{104} A more sophisticated calculation by Morf,\textsuperscript{105} taking into account the downward renormalization of $\mu(T)$ from its $T = 0$ value, agrees with the measured value of $\Gamma_m$.\textsuperscript{101} Unfortunately, with this system, the question of the existence of a hexatic fluid phase could not be addressed, as there are no signals of a hexatic fluid in this system.

In 1987, Murray and Van Winkle\textsuperscript{106} examined colloidal suspensions of charged polystyrene spheres of diameter approximately 0.30 μm. When confined between glass plates, separated by 1 – 4 μm, in a solution of the correct salt concentration, these spheres form a hexagonal lattice, which can be seen with a microscope, the images digitized, and the structure function $S(q)$ calculated. At the widely spaced end of the wedge, the spheres form a well defined hexagonal solid, and, at the thin end, the diffraction pattern is a uniform ring of an isotropic $2D$ fluid. In the intermediate regime, the diffraction pattern has a hexagonal modulation, consistent with a hexatic phase. The visual data of this experiment is consistent with the KTHNY scenario, but is not definitive.

In 1995, an ingenious refinement was attempted\textsuperscript{107} by confining an uncharged colloidal suspension between two glass plates. A static electrostatic field between them induces an electric dipole moment on the neutral polystyrene spheres, which repel each other. The electric dipole moment, $p_s$, induced on a dielectric sphere of radius $r_0$, and dielectric constant $\epsilon_s$, by
an electric field $\mathbf{E}$ in a medium of dielectric constant $\epsilon_m$, is

$$p_s = -\frac{\epsilon_m(\epsilon_m - \epsilon_s)}{2\epsilon_m + \epsilon_s} \epsilon_0^3 E.$$  \hspace{1cm} (1.134)

Assuming that the dipoles are all oriented in the same direction, normal to the confining glass plates, leads to a repulsive dipole–dipole energy,

$$V(r) = \epsilon_m \left( \frac{\epsilon_m - \epsilon_s}{2\epsilon_m + \epsilon_s} \right)^2 \left( \frac{r_0}{r} \right)^3 \frac{r_0^3 E^2}{r^3}.$$  \hspace{1cm} (1.135)

The effective interaction strength, $V(r)$, between particles can be controlled by varying the applied electric field $E$ normal to the glass plates. Data on the particle configurations were collected by viewing with a CCD camera, and recording the signal for analysis.

The results of this investigation are consistent with the KTHNY scenario, since melting is observed to occur by a two-stage process, with an intermediate hexatic phase. The exponent, $\eta_{G_0}(T)$, is estimated to be very close to the predicted value of $1/3$ at melting of the solid to hexatic and, at the hexatic to isotropic transition, the data is consistent with the predicted value, $\eta_6 = 1/4$. However, this investigation suffered from difficulties of equilibration, and these measurements were actually done as the system was evolving towards equilibrium, but are in agreement with previous studies. A more serious difficulty is the confining glass plates, which, inevitably, have random trapped electric charges and dipoles. The resulting random pinning potential has all sorts of undetermined effects on the trapped colloid monolayer. However, the three predicted phases, periodic solid, hexatic, and isotropic fluid, are observed, which do agree with theory.

More recent experiments, carried out by Maret and coworkers, from 1999–2006, on colloidal films trapped at the water–air interface of an inverted droplet, have provided data which agree, in almost every respect, with the predictions of the theory of $2D$ melting, which seem to confirm the KTHNY dislocation theory of melting in $2D$. The electric dipoles induced on the polystyrene spheres are replaced by doping the colloidal particles with superparamagnetic $\text{Fe}_2\text{O}_3$, and the external electric field, $E$, is replaced by an applied magnetic field, $H$, normal to the colloidal film. The doped colloidal spheres are denser than water and are trapped at the water–air interface, which is extremely flat and contains no trapped immobile magnetic moments. This substrate is well characterized and very uniform, so this system is a very good realization of an ideal smooth flat substrate, leading to an experimental realization of an isolated two-dimensional system of interacting spherically symmetric particles, that is very close to the theoretical
conditions. Surprisingly, despite the apparently ideal substrate, which has no pinning centers, equilibrating this very small 2D system proves to be surprisingly difficult, and time consuming.\textsuperscript{110} Equilibration is vital because the experiments are designed to check the analytic theory, which is based on equilibrium statistical mechanics. The experiment must obey the theoretical conditions for the comparison to have meaning! Several days, combined with oscillating the magnetic field, are needed. The positions of the colloidal particles are tracked by a CCD camera, recorded and analyzed in detail. In these experiments, the interaction strength $\Gamma$ is given by\textsuperscript{72}

$$\Gamma = \frac{\mu_0 \chi^2 H^2 (\pi \rho)^{3/2}}{k_B T} \propto \frac{1}{T_{\text{eff}}},$$

(1.136)

where $H$ is the magnetic field normal to the plane of the film, $\chi$ the susceptibility per particle, and $\rho$ the area number density of particles. The particle–particle interaction,

$$\frac{V(r)}{k_B T} = \frac{\Gamma}{(r/r_0)^3} \text{ where } r_0 = (\pi \rho)^{-1/2},$$

(1.137)

is controlled by the magnetic field, $H$. The whole film contains up to $3 \times 10^5$ particles of which, typically, $3 \times 10^3$ are in the field of view. The water–air interface is kept flat to within 250 nm by controlling the amount of water in the inverted droplet.\textsuperscript{72}

Overall, the results from these experiments agree quantitatively with the predictions of the KTHNY theory of melting, finding a power law decay of the positional correlation function for $\Gamma \geq \Gamma_m$,

$$C_{G_0}(r) \sim r^{-\eta_{G_0}(T)},$$

(1.138)

with the exponent $\eta_{G_0}(T) = 1/3$ at $T_m$, and decreasing as $T$ decreases, as expected. Also, for $T > T_m$, the positional correlation function is observed to decay faster than any power as $r$ increases, consistent with the predicted exponential behavior of Eq. (1.103).\textsuperscript{98} Also, the elastic moduli, $\mu_R(T)$, $\lambda_R(T)$, and the Young’s modulus, $K_R(T)$, are measured,\textsuperscript{111} and found to agree remarkably well, for $T \leq T_m$, with the theoretical predictions of Nelson and Halperin.\textsuperscript{42}

Knowing the individual positions of every particle in the field of view, enables one to study, quantitatively, the orientational order by calculating the orientational correlation function,\textsuperscript{112} which is just the two-point correlation
function of the planar rotor model, Eq. (1.55),
\[
G_6(r) = \langle \psi_6(r) \psi_6^*(0) \rangle ,
\]
\[
\psi_6(r) = \psi_k = \frac{1}{N_k} \sum_j e^{6i\theta_{jk}} ,
\]
(1.139)
where \( r \) is the position of the particle \( k \), and \( \theta_{jk} \) is the angle between a fixed reference axis and the bond between particles \( k \) and \( j \). The average is over all nearest neighbor particle pairs for each image, but also over many independent images. Theory predicts that
\[
G_6(r) \neq 0 , \quad r \to \infty , \quad T \leq T_m ,
\]
\[
G_6(r) \sim r^{-\eta_6(T)} , \quad T_m < T \leq T_I ,
\]
\[
G_6(r) \sim e^{-r/\xi_6(T)} , \quad T > T_I.
\]
(1.140)
The orientational correlation length, \( \xi_6(T) = \exp \left( b|\Gamma^{-1} - \Gamma_I^{-1}|^{-1/2} \right) \), and the exponent, \( \eta_6(\Gamma) \), is related to the Frank constant, \( K_A(\Gamma) \), as,
\[
\eta_6(\Gamma) = \frac{18k_B T}{\pi K_A(\Gamma)} .
\]
(1.141)
As we have seen, \( \eta_6(\Gamma_I) = 1/4 \), and, just above the melting temperature \( T_m \),
\[
K_A(\Gamma) \sim \xi_6^2 \sim \exp \left( \frac{2b}{|\Gamma^{-1} - \Gamma_I^{-1}|^\nu} \right) ,
\]
(1.142)
where \( \nu = 0.3696 \cdots \). The data fit these theoretical expressions up to \( r/a = 30 \) rather well, and can be considered as very strong evidence for the dislocation unbinding mechanism of melting, followed by a disclination unbinding transition between an intermediate hexatic fluid, with finite orientational stiffness and algebraic order, to an isotropic fluid at \( T_I > T_m \).

Despite the rather good fits of the experimental data to all the theoretical predictions of the dislocation theory, one cannot exclude the possibility that weakly first order transitions preempt the continuous transitions of theory. For example, if the discontinuity in the Young’s modulus at the melting temperature, \( T_m \), turns out to be just slightly larger than the universal value,
\[
\lim_{T \to T_m} K_R(T) = 16\pi ,
\]
(1.143)
the theoretical continuous transition must be preempted by a first order melting transition. A similar discussion holds for the hexatic–isotropic transition. The available experimental data, although very good, is not sufficiently detailed, nor of sufficient resolution to exclude a weak first order
transition. Perhaps, in the future, a smoking gun will be discovered which is capable of distinguishing between a weak first order melting transition and the continuous melting transition of KTHNY theory. At least, in the paramagnetic colloid system of Maret and coworkers,\textsuperscript{72} the data agree quantitatively, to within experimental resolution, with all theoretical predictions of the KTHNY topological defect theory, and is completely consistent with two continuous transitions.

There have also been some experimental studies of anisotropic colloidal crystals in 2D,\textsuperscript{110,113} by tilting the magnetic field away from the normal to the plane of the colloidal system. This tilt modifies the interaction between particles from an isotropic \(1/r^3\) interaction, when the magnetic field, \(H\), normal to the droplet interface to an anisotropic dipole–dipole interaction,

\[
V(r) = \frac{\mu_0(\chi H)^2}{8\pi r^3}(1 - 3(\hat{H} \cdot \hat{r})^2),
\]

(1.144)

where \(\hat{H}\) and \(\hat{r}\) are unit vectors in the direction of the field \(H\) and the separation \(r\) respectively. For small angles of tilt, a two-step melting process of a distorted hexagonal lattice is observed. For larger angles of tilt, the equilibrium crystal phase is a very anisotropic centered rectangular lattice, which melts into a 2D smectic-like phase.\textsuperscript{113} This is similar to theoretical expectations for dislocation mediated melting of anisotropic layers.\textsuperscript{114,115}

### 1.7.3. Simulations of 2D melting

There have been a number of numerical simulations of 2D melting on a smooth substrate. Alder and Wainwright’s study of hard discs in 1962,\textsuperscript{124} on the basis of a van der Waals loop in the pressure, claimed that the melting of this system is of first order. As bigger, better, and faster computers became available, larger and larger arrays of discs were simulated, but the first order/continuous melting controversy escalated, instead of settling to an agreed answer.\textsuperscript{97} Most early simulations on hard discs, or on discs with a \(1/r^3\) repulsion, failed to identify a hexatic phase, and concluded that melting was a direct first order transition, with supercooling and superheating, from a solid phase to an isotropic fluid.\textsuperscript{125–129} There was also no consensus about the mechanism of melting in the hard disc system.\textsuperscript{130–132} Bagchi \textit{et al.}\textsuperscript{133} did a finite size analysis of bond orientational order in a system of particles interacting with a repulsive \(1/r^{12}\) interaction and found agreement with KTHNY theory. However, conclusive evidence for a hexatic phase was not found. Jaster, in a series of large scale simulations of the hard disc system,\textsuperscript{134–136} obtained good agreement with theory for the melting transition,
and some evidence for the existence of a hexatic phase, but the expected algebraic decay of the orientational correlation function was missed. Simulations of an electron system with a $1/r$ interaction did find algebraic decay of the correlation function, $^{137}$ successfully demonstrating the existence of the hexatic phase. Finally, Lin et al. $^{138}$ performed a finite size scaling analysis of a system of up to $N = 16384$ particles, with a dipole–dipole interaction, succeeded in fitting their data to KTHNY theory for both positional and orientational correlations. At about the same time, Mak $^{139}$ performed a simulation of up to $N = 2048^2$ hard discs, and demonstrated, by a finite size scaling analysis, that the van der Waals loops at the two transitions seem to scale away. This is consistent with both the solid–hexatic and the hexatic–isotropic transitions being continuous, and a van der Waals loop being a finite size artifact. However, there seems to still be some uncertainty about the isotropic–hexatic transition in the $2D$ hard disc system. $^{139}$

An important contribution to simulations of $2D$ melting was made by Saito, $^{140}$ who performed Monte Carlo simulations on the dislocation Hamiltonian part, $H_D$, of Eq. (1.93), allowing the core energy, $E_c$, to be an independent parameter. The positions of the Burgers vector variables, $b(r)$, lie on the sites, $r$, of a triangular mesh of size up to $N = 1762$ points. The simulation is carried out in a rectangular box of size $\Omega = L_x L_y$, with periodic boundary conditions. The mesh site $r = (x, y) = a(l, \sqrt{3}m)$, with $0 \leq l < L = L_x/a$ and $0 \leq m < L_y/a\sqrt{3}$, with $l + m$ even. The Burgers vectors are restricted to their six smallest values, $b = (\pm a_0, 0), (\pm a_0/2, \pm \sqrt{3}a_0/2)$. The simulations, with a large core energy, $E_c$, are consistent with a continuous KTHNY melting transition. $^{140}$ On the other hand, the simulation data for small core energy, $E_c$, is more consistent with a first order transition. Interestingly, a study of the distribution of dislocations indicates that they are organized into grain boundaries, for small $E_c$, which is consistent with the grain boundary melting picture of Chui. $^{141}$ These simulations are unable to study the hexatic phase or the hexatic/isotropic transition, as the essential disclinations are excluded in the dislocation Hamiltonian of Eq. (1.93).

The first order versus continuous transition controversy led to the introduction, in 1982, of the Laplacian roughening model. $^{142}$ This model, defined on a triangular lattice, is dual to a melting model of interacting disclinations. The variables are a set of integer valued heights, $-\infty < h(r) < +\infty$, with Hamiltonian,

$$H = -\frac{J}{2} \sum_r \left( \frac{2}{3} \sum_{i=1}^{6} (h(r + \delta_i) - h(r)) \right)^2, \quad (1.145)$$
where $\delta_i$ is an elementary lattice vector. By using the Poisson summation formula,\(^{143}\)

\[
\sum_{h=-\infty}^{+\infty} f(h) = \sum_{s=-\infty}^{+\infty} \int_{-\infty}^{+\infty} dh f(h) e^{2\pi i sh},
\]

in the partition function, one obtains,

\[
Z = \prod_r \sum_{h(r)} e^{-\beta H[h]} = \prod_r \sum_{s(r)} \int_{-\infty}^{+\infty} dh(r) \exp \left( -\beta H(h) + 2\pi i \sum_r s(r)h(r) \right),
\]

\[
\propto \sum \{ s(r) \} \exp \left( \frac{2\pi^2 k_BT}{J} \sum_{r \neq r'} V(r-r')s(r)s(r') \right),
\]

\[
\propto \sum \{ s(r) \} \exp \left( \frac{K}{16\pi} \sum_{r \neq r'} |r-r'|^2 \ln|r-r'|s(r)s(r') + E_c \sum_r s^2(r) \right),
\]

\[
V(r) \approx \frac{1}{8\pi} (r^2 \ln r + Ar^2 - B), \quad K = \frac{4\pi^2 k_BT}{J}, \quad E_c = \frac{B K}{16\pi}.
\]

In the dual representation, the integer variable, $s(r)$, is the strength of a disclination at site $r$. These are subject to neutrality conditions, $\sum_r s(r) = 0 = \sum_r rs(r)$. In the disclination representation, $E_c$ represents the core energy of a disclination, which also determines the core energy of a dislocation, as a dislocation can be regarded as a disclination dipole.\(^{142}\)

One can change $E_c$ from its value obtained from the pure nearest neighbor roughening model of Eq. (1.145) by adding some further neighbor interactions to this Hamiltonian.\(^{144,145}\) Strandburg\(^{145}\) made a series of simulations on a modified Laplacian roughening model, designed to test the effect of the size of the dislocation and disclination core energies on the order of the 2D melting transitions. There have been some numerical studies on the effects of lowering the vortex core energy on the transition in the planar rotor model\(^{146-148}\) with the conclusion that the continuous KT transition of Sec. 1.5 becomes first order when the defect core energy is sufficiently small. However, another study of the roughening representation of a 2D planar rotor model coupled to an Ising degree of freedom, where the two transitions could merge to become a single first order transition, showed that the first order transition did not occur, but the two second order lines came very close to each other.\(^{149}\) One might speculate that reducing the defect core
energy might make the hexatic phase disappear resulting in a direct first order transition from a periodic solid to an isotropic fluid. The simulations by Strandburg\textsuperscript{144,145} are designed to test this hypothesis. The simulations were performed on a Laplacian roughening model on a triangular lattice described by a Hamiltonian,

$$H[h] = \sum_{\mathbf{q}} [G^{\mathbf{q}} - 2G^{-\mathbf{q}}h(\mathbf{q})h(-\mathbf{q})]$$

where $\gamma = \sqrt{3}/\delta E_c$ and $\delta E_c$ is the change in the dislocation core energy.

The results of these simulations are, for the disclination core energy $E_c > E_c^* \approx 2.7$, the duals of the three phases predicted by theory\textsuperscript{42} are clearly visible, with quantitative agreement with theory. For the core energy, $E_c < E_c^*$, the two transitions seem to merge into a single first order transition.\textsuperscript{145} These simulations are in accord with expectations, with the caveat that it is possible that the separation between the two transition lines becomes so small that they look like a single first order transition.

References

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Early Work on Defect Driven Phase Transitions

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