Melting and the vector Coulomb gas in two dimensions

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The dislocation theory of two-dimensional melting due to Kosterlitz and Thouless is investigated for the triangular lattice, paying special attention to angular forces between dislocation pairs, which are equal in magnitude to the radial forces. Generalizing the dislocation Hamiltonian to an arbitrary vector Coulomb gas with different radial and angular interactions we find $K_R^i(T)-K_R^i(T_c^-)\sim t^{\bar{\nu}}$, where K_R^i is a renormalized coupling which includes the screening effect of bound dislocation pairs, the superscript i signifies either a radial, r, or angular, θ part and t is the reduced temperature, $t=(T_c-T)/T_c$. The exponent $\bar{\nu}$ varies as the ratio $K_R^\theta(T_c^-)/K_R^r(T_c^-)$ is changed and is equal to 0.3696··· for the physical value of $K^\theta = K^r$. In this case the shear and bulk elastic constants have the same temperature dependence as the K_R^i. We find that K_R^r has finite universal value at T_c and $K_R^i = 0$ for $T > T_c$, corresponding to metallic behavior of the vector Coulomb gas.

I. INTRODUCTION

Kosterlitz and Thouless[1] have proposed a theory for a phase transition in two-dimensional planar spin systems and helium films, and for two-dimensional melting. These systems have singularities, vortices for planar spins and helium, dislocations in the case of melting, which interact with a logarithmic potential. At low temperature they occur in tightly bound pairs, but at sufficiently high temperature it is favorable for the pairs to dissociate because of the resulting gain in entropy. Subsequently Kosterlitz[2] carried out a renormalization-group calculation for the planar magnet which gives equivalent results.[3]

Long-range positional order does not occur for a two-dimensional solid[4] and in a harmonic approximation, neglecting dislocations, the correlation function $\langle e^{i\vec{G}\cdot\vec{u}(0)}e^{-i\vec{G}\cdot\vec{u}(r)}\rangle$ decays at large distances with a power law,[5] the exponent depending continuously on temperature. Here $\vec{G}$ is a reciprocal-lattice vector and $\vec{u}(\vec{r})$ the displacement at point $\vec{r}$. In the Kosterlitz-Thouless theory the harmonic approximation is exact at all temperatures below the transition temperature T_c, provided one only investigates fluctuations on a sufficiently large length scale and allows for a renormalization of the elastic constants due to bound dislocation pairs. Above T_c correlations are expected to decay exponentially with a correlation length of order of the mean spacing between free dislocations.

A criterion for distinguishing between a solid and a liquid is that a solid exhibits resistance to shear, characterized by a shear modulus μ. When dislocations appear only in tightly bound pairs the material has a nonzero shear modulus so we denote the low-temperature phase of the Kosterlitz-Thouless theory as a solid. However, when free dislocations appear the system will respond to a shear stress with no resistance by continuously creating dislocation pairs and pulling them apart to infinity. It is therefore tempting to call the phase above T_c a liquid. In fact it has recently been shown[10] that this phase resembles a two-dimensional liquid crystal characterized by power-law decay of angular correlations. A subsequent transition at higher temperature involving an unbinding of disclination pairs is required to complete the melting process. In this paper we discuss only the solid phase at temperatures up to and including T_c.

In the Kosterlitz-Thouless theory one neglects interactions between dislocations and harmonic lattice vibrations and evaluates the energy of the dislocation system $\mathcal{H}_D$ using continuum elasticity theory.[6] Defining $H_D=-\mathcal{H}_D/k_BT$ one finds

$$H_0 = 2\pi \sum_{\langle ij\rangle} \{K_0^r \vec{b}^i\cdot\vec{b}^j \ln(r^{ij}/a_0) - K_0^\theta[(\vec{b}^i\circ\vec{r}^{ij})(\vec{b}^j\cdot\vec{r}^{ij})/(r^{ij})^2 - \tfrac{1}{2}\vec{b}^i\circ\vec{b}^j]\} + \ln y_0 \sum_i (b^i)^2 , \quad (1)$$

where $\vec{r}^{ij}=\vec{r}^i-\vec{r}^j$, $\vec{r}^i$ denotes the position of the ith dislocation with dimensionless Burger vector $\vec{b}^i$, $\ln y_0$ is related to the core energy, and a_0 is the lattice spacing. The dislocations are located on the sites of the dual lattice (which is hexagonal if the original lattice is triangular; the square lattice is self-dual) and satisfy the condition $\sum_i \vec{b}^i=0$. The summation over pairs $\langle ij\rangle$ in (1) assumes $i\neq j$ and counts each pair just once. $K_0^r=K_0^\theta=K_0$ with

$$K_0 = \frac{1}{2\pi^2}\,\frac{\mu_0 B_0}{\mu_0+B_0}\,\frac{a_0^2}{k_BT} , \quad (2)$$

where μ_0 and B_0 are the shear and bulk moduli in the absence of dislocations. We shall later consider a generalization of (1) where $K_0^r\neq K_0^\theta$. B_0 is

related to μ_0 and the Lamé coefficient λ_0 by $B_0 = \mu_0 + \lambda_0$. We have defined K_0 in this way so that our notation is as close as possible to that of Ref. 7. The Burger vectors have the form $\vec{b} = m\vec{e}_1 + n\vec{e}_2$, where n and m are integers and $\vec{e}_1$ and $\vec{e}_2$ are unit vectors of the Bravais lattice. Our discussion will be restricted to the square and triangular lattices. Strictly Eqs. (1) and (2) do not apply to the square lattice which is characterized by three elastic constants[8] and this will lead to some complications later on. We expect that the angular dependence of the interactions would be different from (1) but that a term of the form $\vec{b} \cdot \vec{b} \ln(r/a_0)$ would remain. Our principal results are for the triangular lattice for which (1) and (2) are correct.

The Hamiltonian (1) corresponds to a vector Coulomb gas and is more complicated than the scalar Coulomb gas which describes vortex dissociation in planar magnets because of the angular interaction K_0^θ. An additional difficulty arises for the triangular lattice because two Burger vectors of unit length can be combined to give another unit vector. If these extra complications are neglected the theory of Refs. 2 and 7 predict that the "renormalized" coupling $K_R(T)$, which differs from K_0 because of screening due to vortex pairs, is given by

$$2\pi K_R(T) = 4 + Ct^{\bar{\nu}} \tag{3}$$

as T approaches T_c from below, where t is the reduced temperature, $t = (T_c - T)/T_c$, the exponent $\bar{\nu}$ is equal to $\frac{1}{2}$, and C is a nonuniversal constant. Notice that $K_R(T_c^-)$ equals the universal[7] value of $2/\pi$. Above T_c, $K_R = 0$.

Nelson[9] has recently discussed two-dimensional melting including the effects of the vector nature of b but with $K_0^\theta = 0$. For the square lattice he finds that Eq. (3) is unchanged, but the triangular lattice he obtains $\bar{\nu} = \frac{2}{5}$ instead of $\frac{1}{2}$, the difference arising from the possibility of combining two unit Burger vectors to give a third unit vector. In this paper we study in detail the role of the angular forces in the Hamiltonian (1). Our conclusion is that $\bar{\nu}$ varies continuously on the triangular lattice as the ratio of radial to angular interaction is changed. For $K_0^\theta = 0$ we recover Nelson's result of $\bar{\nu} = \frac{2}{5}$ whereas in the physical case with $K_0^\theta = K_0^r$ we obtain $\bar{\nu} = 0.3696\cdots$. After the bulk of this work was completed we received a preprint from Halperin and Nelson[10] who have evaluated $\bar{\nu}$ for $K_0^\theta = K_0^r$ obtaining the same result as given here. They also point out that phase transitions on a substrate can be described by the Hamiltonian (1) but with $K_0^\theta \neq K_0^r$. We therefore feel that our evaluation of $\bar{\nu}$ for arbitrary values of the parameters is of some physical interest. We do not give a complete discussion for the square lattice but expect that $\bar{\nu} = \frac{1}{2}$ for arbitrary values of the parameters on the dislocation Hamiltonian.

For the case of $K_0^r = K_0^\theta (= K_0)$ we follow Kosterlitz and Thouless and introduce a scale-dependent dielectric constant $\epsilon(r)$ which includes the screening effect of dislocation pairs of separation between a and r. Below T_c, $\epsilon(\infty)$ is finite and the renormalized coupling $K_R(T)$ introduced above is given by

$$K_R = K_0/\epsilon(\infty). \tag{4}$$

The same linear-response theory also permits an evaluation of the elastic constants which similarly have renormalized values $\mu_R(T)$ and $B_R(T)$ different from μ_0 and B_0 because of screening effects. As pointed out by Nelson and Halperin[10] there are additional contributions to the bulk, but not the shear, elastic modulus arising from creation of vacancies and interstitials. The true bulk modulus differs therefore from our $B_R(T)$ and is expected to have a very different temperature dependence in the transition region.[10] At $T = T_c$ we find that K_R has the universal value of $2/\pi$ while μ_R and B_R have finite nonuniversal values.

We investigate screening in the general vector Coulomb gas with $K_0^r \neq K_0^\theta$ by Kosterlitz's renormalization-group approach. The exponent $\bar{\nu}$ is now nonuniversal but $K_R(T_c^-)$ still has the universal value of $2/\pi$ suggested by Kosterlitz and Thouless' entropy argument. It is also possible to derive the renormalization-group equations from the model discussed by Halperin and Nelson of melting on a periodic substrate where the adsorbed layer is characterized by three elastic constants (which do not correspond to the three elastic constants for the square lattice) and a dislocation Hamiltonian with $K_0^r \neq K_0^\theta$. That the results of the two approaches are identical provides a useful self-consistency check on the calculations.

The linear-response theory is explained in Sec. II and in Sec. III the exponent $\bar{\nu}$ is evaluated for $K_0^r = K_0^\theta$. In Sec. IV we show how to evaluate $\bar{\nu}$ for $K_0^r \neq K_0^\theta$ and discuss our results in Sec. V. The linear-response theory for elastic constants is given in Appendix A while in Appendix B we show how to derive renormalization-group equations for $K^r \neq K^\theta$ from an elasticity theory with three elastic constants.

II. SELF-CONSISTENT INTEGRAL EQUATION

In this section we take $K_0^r = K_0^\theta = K_0$ and discuss how K_0 is renormalized by dislocation pairs within a linear-response formalism. First of all we will discuss the square lattice neglecting angular forces. Then the angular forces will be included and finally the more complicated case of the tri-

angular lattice is discussed.

Only Burger vectors of unit length will be considered. At the end of the calculation it will be clear that including larger Burger vectors would not change the results in the critical region. If the angular forces are neglected the Burger vectors in the x and y directions on the square lattice are independent and can be considered as two sets of (scalar) vortices. There is a direct correspondence between plus and minus vortices interacting via a logarithmic potential and a two-dimensional neutral Coulomb gas of charges $\pm q$. Taking the basic equation of electrostatics to be Poisson's equation $\nabla^2\phi = -4\pi\rho$ we find that in two dimensions the potential between two charges q_i and q_j is $-2q_iq_j\ln(r_{ij}/a_0)$ and comparing with (1) we make the correspondence

$$\pi K_0 = q^2/k_BT . \tag{5}$$

Consider a pair of opposite charges with separation r where $r \gg a$. The force, which is just the electric field E divided by the charge is reduced from its "bare" value $2\pi K_0/r$ by the screening effect of *smaller* dipoles. Kosterlitz and Thouless treat the smaller dipoles as a continuous medium so they can take over dielectric theory, the basic equations of which are

$$E = D/\epsilon , \tag{6a}$$

$$\epsilon = 1 + 4\pi\chi , \tag{6b}$$

where ϵ is the dielectric constant, χ the susceptibility, and D is the field that would be present if the material were not polarizable and is due to some external test charges, in our case the pair separated by r. Clearly the reduction in force depends on the separation r so Kosterlitz and Thouless introduce a scale-dependent dielectric constant $\epsilon(r)$ such that the force is $2\pi K_0/r\epsilon(r)$, which we also write as $2\pi K(r)/r$, where

$$\epsilon(r) = 1 + 4\pi\chi(r) \tag{7}$$

and $\chi(r)$ is susceptibility of all dipoles of separation less than r. $\chi(r)$ is then given by

$$\chi(r) = \int_a^r n(r',\theta)\alpha(r')r'\,dr'\,d\theta , \tag{8}$$

where $\alpha(r')$ is the polarizability of a single dipole of separation r', which is[1]

$$\alpha(r') = \tfrac{1}{2}(q^2/k_BT)(r')^2 = \tfrac{1}{2}\pi K_0(r')^2 , \tag{9}$$

where the last line follows from (5). $n(r',\theta)$ is the density of pairs separated by r', where the dipole makes an angle θ with some axis and must be evaluated from (1) recognizing that the interaction between the pairs is modified from $2\pi K_0\ln(r'/a_0)$ because of the screening effect of still smaller pairs. The energy is obtained from integrating up the force and we write it as $U(r')\ln(r'/a_0)$, where

$$U(r')\ln(r'/a_0) = K_0\int_{\ln a}^{\ln r'} \frac{d\ln r''}{\epsilon(r'')} . \tag{10}$$

To leading order in y_0^2 it is now straightforward to show that

$$n(r',\theta) = (y_0/a_0^2)^2(r'/a_0)^{-2\pi U(r')} . \tag{11}$$

Combining Eqs. (7)–(11) it follows that

$$\epsilon(r) = 1 + 4\pi^3y_0^2K_0\int_a^r \left(\frac{r'}{a_0}\right)^{4-2\pi U(r')}\frac{dr'}{r'} , \tag{12}$$

which is a *self-consistent* equation for $\epsilon(r)$ and is the central result of the Kosterlitz-Thouless theory. It is useful to rewrite (12) as an equation for $K(r)[=K_0/\epsilon(r)]$ and let $l = \ln(r/a_0)$ after which one finds

$$K^{-1}(l) = K_0^{-1} + 4\pi^3y_0^2\int_0^l \exp\left(4l' - 2\pi\int_0^{l'} K(l'')dl''\right) . \tag{13}$$

As pointed out in Ref. 3 it is useful to unravel the double integral in (13) by defining an auxiliary variable

$$y(l) = y_0\exp\left(2l - \pi\int_0^l K(l')\,dl'\right) \tag{14}$$

so that (13) is equivalent to the pair of coupled differential equations

$$\frac{dK^{-1}}{dl} = 4\pi^3y^2 , \tag{15a}$$

$$\frac{dy}{dl} = (2 - \pi K)y , \tag{15b}$$

which are the scaling equations of Kosterlitz.[2]

For $T > T_c$ $\epsilon(r\to\infty)$ diverges as discussed in Sec. I so from (12) we see that T_c is characterized by $U(r\to\infty) = 2/\pi$, which also corresponds[3] to $K(r=\infty) = 2/\pi$ [see Eq. (3)]. For $T = T_c$ the left-hand side of (12) is $K_0/K(r)$ which is finite for $r\to\infty$ and the right-hand side is also finite because $U(r)$ approaches its asymptotic value for large r sufficiently slowly such that the integral in (12), which has a potential logarithmic divergence, actually converges.[3] This example makes clear the importance of having a self-consistent theory and inserting the *scale-dependent* potential $U(r')$ in the exponent inside the integral of (12).

In order to carry out a similar analysis for the full dislocation problem including the angular forces, it is necessary to generalize the above linear-response theory to a vector Coulomb gas. Kosterlitz and Thouless[1] have discussed such a theory and concluded that the main change is that

the polarizability $\alpha(r')$ is modified from Eq. (9) and now reads

$$\alpha(r') = \tfrac{1}{2}\pi K_0(r')^2(1 - \tfrac{1}{2}\langle\cos 2\theta\rangle_{\text{ang}}), \tag{16}$$

where θ is the angle the displacement vector between a pair of opposite Burger vectors makes with the Burger vectors and the angular average is over $\exp[\pi K(r')\cos 2\theta]$ which comes from (1). In the Appendix we derive (10) from a somewhat different form of linear-response theory[10] which permits, in addition, a calculation of the renormalized elastic constants. Like Eq. (1) the linear-response theory is strictly incorrect for the square lattice. However, we shall apply it as it stands and argue that a more exact treatment would not change the results. $n(r,\theta)$ is multiplied by a factor 2 to account for there being two species of pairs of opposite Burger vectors for the square lattice (this factor will be 3 for the triangular lattice) and also includes the part of the Gibbs distribution coming from the angular interaction $\exp[\pi K(r')\cos 2\theta]$.

Consequently we find, to leading order in y_0^2,

$$n(r',\theta) = 2(y_0/a_0^2)^2 \exp[\pi K(r')\cos 2\theta] \times (r'/a_0)^{-2\pi U(r')}. \tag{17}$$

Combining (7), (8), (16), and (17) and carrying out the angular integration one obtains

$$K^{-1}(l) = K_0^{-1} + 8\pi^3 y_0^2 \int_0^l [I_0(\pi K) - \tfrac{1}{2} I_1(\pi K)] \times \exp\left[4l' - 2\pi \int_0^{l'} K(l'')dl''\right] dl', \tag{18}$$

which is equivalent to the differential equations

$$\frac{dK^{-1}}{dl} = 8\pi^3 y^2 [I_0(\pi K) - \tfrac{1}{2} I_1(\pi K)], \tag{19a}$$

$$\frac{dy}{dl} = (2 - \pi K)\, y, \tag{19b}$$

where I_0 and I_1 are modified Bessel functions and $y(l)$ is defined in (14). Equations (19) are our recursion relations for the square lattice including the angular interaction approximately. Comparing (13) and (19) we see that the change induced by the angular forces can be compensated for by a redefinition of y. We expect that the same would be true if the angular interactions were included exactly and conclude that they do not change the value of the exponent $\bar{\nu}$ for melting on the square lattice. Equation (18) corresponds closely to Eq. (81) of Kosterlitz and Thouless[1] except that they replace $\int_0^{l'} K(l'')\,dl''$ by $l'K(l')$ and have a different coefficient in front of the integral.

Two modifications have to be made to Eq. (18) in the calculation for the triangular lattice. First of all there are three species of pairs of oppositely oriented Burger vectors as opposed to two for the square lattice. As a result the prefactor 2 in Eq. (17) for $n(r',\theta)$ is replaced by 3 with the result that the coefficient of the integral in (18) is $12\pi^3$ instead of $8\pi^3$. The second modification is less trivial and arises because two Burger vectors, for example, in orientations ↖ and ↗, can be combined to give one Burger vector in direction ↑.

In the dielectric theory described above we replaced the pairs of oppositely pointing Burger vectors with separation r' less than the separation r of a test pair by a continuous medium. In the same spirit we ignore the "structure" in the pair ↖↗ provided they are separated by a distance $r' < r$ and consider them to be a single Burger vector with orientation ↑. This means that y_0 in (18) must be modified to include these "composite" Burger vectors. To be precise, for the pair separated by r' which is doing the screening, we have to allow for the possibility that either of them may be a composite Burger vectors of separation $r'' < r'$. We therefore replace y_0 by $\bar{y}(r')$ in (17) and proceed to evaluate $\bar{y}(r')$.

To lowest order in y_0, $\bar{y}(r')$ is just y_0 plus the probability that there is a pair of type ↖↗ with separation $r' < r'$ and is

$$\bar{y}(r') = y_0 + y_0^2 \int_a^{r'} \left(\frac{r''}{a_0}\right)^{2-\pi U(r'')} \times \exp[\pi K(r'')\cos 2\theta]\, d\theta\, \frac{dr''}{r''}, \tag{20}$$

where θ is the angle made by the displacement between the pair relative to the direction of the composite Burger vector. As T goes through T_c the integral in (20) diverges so the correction, although of order y_0^2, is not small. To rectify this difficulty the theory must be made self-consistent with respect to $\bar{y}(r)$ just as we handled correctly the divergence of the integral in (12) by making it self-consistent with respect to $K(r)$. In a self-consistent theory we recognize that either of the Burger vectors making the composite Burger vector could itself be composed of two Burger vectors of still smaller separation. Thus y_0^2 in (20) should be replaced by $\bar{y}^2$ appropriate to length scale r'' and put inside the integral. In this way (20) is replaced by

$$\bar{y}(l) = y_0 + 2\pi \int_0^l \bar{y}^2(l') I_0(\pi K) \times \exp\left(2l' - \pi \int_0^{l'} K(l'')\, dl''\right) dl', \tag{21}$$

which is equivalent to the differential equation

$$\frac{d\bar{y}}{dl} = 2\pi I_0(\pi K)\exp\left(2l - \pi\int_0^l K(l')\,dl'\right) y^2(l). \quad (22)$$

Now that we have obtained a self-consistent expression for $\bar{y}(l)$, we replace y_0 by $\bar{y}(l')$ in (18) inside the integral, and find that the analog of (18) for the triangular lattice is

$$K^{-1}(l) = K_0^{-1} + 12\pi^3\int_0^l \bar{y}^2(l')[I_0(\pi K) - \tfrac{1}{2}I_1(\pi K)] \times \exp\left(4l' - 2\pi\int_0^{l'} K(l'')dl''\right) dl'. \quad (23)$$

Defining

$$y(l) = \bar{y}(l)\exp\left(2l - \pi\int_0^l K(l')\,dl'\right), \quad (24)$$

Eq. (23) is equivalent to

$$\frac{dK^{-1}}{dl} = 12\pi^3 y^2[I_0(\pi K) - \tfrac{1}{2}I_1(\pi K)] \quad (25a)$$

and from (22) and (24) we find that y satisfies the equation

$$\frac{dy}{dl} = (2 - \pi K)y + 2\pi I_0(\pi K)y^2. \quad (25b)$$

Equations (25a) and (25b) are our final recursion relations for the triangular lattice.

Neglecting the angular force corresponds to setting the argument of the Bessel functions equal to zero and dividing the coefficient on the right-hand side of (25a) by 2. This factor of 2 arises because the radial force and the angular force give equal contributions to the "polarizability" in Eq. (10). One then recovers the scaling equations of Nelson.[9]

Because of the second term on the right-hand side of (25b) the factors involving Bessel functions cannot be transformed away by a redefinition of y as is possible with (19). This term arises from the possibility, unique to the triangular lattice, of combining two unit Burger vectors to form another unit Burger vector, and so cannot occur for the square lattice even with an exact treatment of the angular interactions.

III. EVALUATION OF THE EXPONENT $\bar{\nu}$

Nelson[9] has discussed the critical behavior implied by equations similar to (25) and our discussion follows his closely. First of all we simplify (25), replacing the arguments of the Bessel functions by 2, their value at $T = T_c$ $l \to \infty$, and by defining

$$x = 2 - \pi K, \quad (26a)$$

$$Y = \pi y I_0(2)/\alpha, \quad (26b)$$

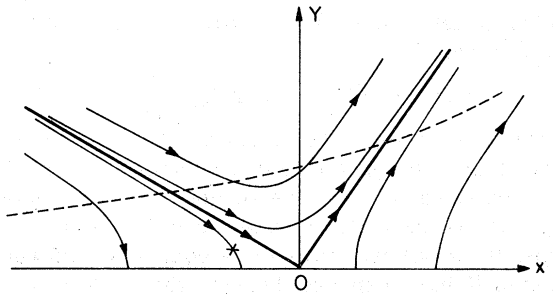

FIG. 1. Schematic drawing of trajectories corresponding to the differential equations (28a) and (28b) of the text. The thick lines (separatrices) have gradients m given by the solutions of the quadratic equation (29). At $T = T_c$ the trajectories flow along the separatrix with negative slope. For $t = (T_c - T)/T_c$ very small and positive the trajectory stays close to the separatrix until one has integrated up the equations to a large value l^*. Beyond this the deviation from the separatrix is large and x does not continue to increase much more. We have indicated by a cross the point on one of the trajectories where $l \sim l^*$. The dashed line indicates a typical locus of starting values (x_0, Y_0).

where

$$\alpha^2 = \frac{I_0(2)}{48}\left(1 - \frac{1}{2}\frac{I_1(2)}{I_0(2)}\right)^{-1} = 0.072\,939\cdots \quad (27)$$

for $x, Y \ll 1$ Eqs. (25) are then equivalent to

$$\frac{dx}{dl} = Y^2, \quad (28a)$$

$$\frac{dY}{dl} = xY + 2\alpha Y^2. \quad (28b)$$

The trajectories which follow from Eqs. (28) are shown schematically in Fig. 1 together with a typical locus of starting values x_0, Y_0. The two solutions which pass through $x = Y = 0$ are straight lines (separatrices) with slope m given by the solutions of the quadratic equation

$$m^2 - 2\alpha m - 1 = 0. \quad (29)$$

We shall be interested in the negative slope and define $m = -m_0$ $(m_0 > 0)$ so

$$m_0 = (\alpha^2 + 1)^{1/2} - \alpha. \quad (30)$$

To the left of the separatrix with negative slope $Y \to 0$ and x goes to a finite negative value as $l \to \infty$, which implies a finite $\epsilon(\infty)$ and hence a solid phase. Elsewhere in the diagram x, $Y \to \infty$ as $l \to \infty$ so $\epsilon(l \to \infty)$ diverges which signifies a vanishing shear modulus. On the critical trajectory (separatrix with negative slope) we find

$$x(l) = \frac{-1}{m_0^2}\frac{1}{l + l_0}, \quad Y(l) = \frac{1}{m_0}\frac{1}{l + l_0}. \quad (31)$$

We now assume that T is just below T_c so

$t=(T_c-T)/T_c \ll 1$ and write

$$Y(l)=-m_0 x(l)-D(l)\,, \tag{32}$$

where $D(0)\sim t$. It is straightforward to show that D satisfies the equation

$$\frac{dD}{dl}=-xD+O(D^2)\,, \tag{33}$$

which has solution

$$D(l)=D(0)\exp\int_0^l |x(l')|\,dl'\,. \tag{34}$$

To leading order in D we replace $x(l)$ by its value on the critical trajectory (31) so (34) becomes

$$D(l)=D(0)(l+l_0)^{1/m_0^2}\,. \tag{35}$$

We use this result to integrate up the recursion relations to a value l^* where the trajectory starts to deviate significantly from the separatrix. We could for instance define l^* by $D(l^*)=\frac{1}{2}Y(l^*)$, the precise value of the coefficient being unimportant. Since $D(0)\sim t$ this gives, from (31) and (35)

$$l^*\sim t^{-\bar\nu} \tag{36}$$

with

$$\bar\nu=m_0^2/(1+m_0^2) \tag{37}$$

at which point

$$x(l^*)\sim Y(l^*)\sim 1/l^*\sim t^{\bar\nu}\,. \tag{38}$$

The exponent $\bar\nu$ will turn out to be the same as in Eq. (3). We cannot use (35) for $l\gg l^*$ because the approximations used to derive it break down. Instead we make the approximation that in this region $x(l)$ does not deviate significantly from $x(l^*)$ and justify that this is self-consistent at the end of the calculation. We therefore replace $x(l)$ by $x(l^*)$ in the equation for dY/dl and neglect the Y^2 term because we are in a region where $Y\ll x$. $Y(l)$ then has the form

$$Y(l)\sim(1/l^*)\exp[-|x(l^*)|l] \tag{39}$$

and inserting this in the equation for x we find

$$x(\infty)-x(l^*)\sim 1/l^*\sim x(l^*)\,, \tag{40}$$

which justifies the above assumption. Consequently we obtain

$$x(\infty)\sim t^{\bar\nu} \tag{41}$$

and from (26a) and (41) we find the "renormalized" stiffness K_R, which is just $K(l=\infty)$, is given by

$$2\pi K_R=4+Ct^{\bar\nu}\,, \tag{42}$$

where C is a nonuniversal constant and $\bar\nu$ is given by (37) with m_0 related to α by (30). Our final result, then, is that

$$\bar\nu=1-\tfrac{1}{2}[1+\alpha^2-\alpha(1+\alpha^2)^{1/2}]^{-1}\,. \tag{43}$$

The exponent $\bar\nu$ varies continuously as the coefficient α in (28b) is changed. In Sec. IV we evaluate α for arbitrary values of K_R^θ and K_R^r. Here we consider only $K^\theta=K^r$ (which holds at all scales l) for which α^2 is given by (27) so

$$\bar\nu=0.3696\cdots\,. \tag{44}$$

It is straightforward to show that the integral equations (A11a) and (A11b) can be converted to recursion relations, analogous to (25), which take the form[10]

$$\frac{k_BT}{a_0^2}\,\frac{d\mu^{-1}}{dl}=3\pi y^2 I_0(\pi K)\,, \tag{45a}$$

$$\frac{k_BT}{a_0^2}\,\frac{dB^{-1}}{dl}=3\pi y^2[I_0(\pi K)-I_1(\pi K)]\,, \tag{45b}$$

and dy/dl is still given by (25b). By repeating the above manipulations one finds

$$\mu_R(T)-\mu_R(T_c^-)=C_\mu t^{\bar\nu}\,, \tag{46a}$$

$$B_R(T)-B_R(T_c^-)=C_B t^{\bar\nu}\,, \tag{46b}$$

where, as before, $\bar\nu=0.3696\cdots$ for the triangular lattice. $\mu_R(T_c^-)$ and $B_R(T_c^-)$ are nonuniversal but Eqs. (2) and (42) show that $\mu_R^{-1}+B_R^{-1}$ has a universal value given by

$$\mu_R^{-1}+B_R^{-1}=a_0^2/4\pi K_BT_c \tag{47}$$

at $T=T_c^-$, which is the analog of the universal jump[7] in ρ_s for helium films.

IV. GENERAL VECTOR COULOMB GAS

Screening in the general problem described by (1) with $K_0^r\neq K_0^\theta$ is conveniently treated by the renormalization-group technique of Kosterlitz.[2] An alternative method which gives identical results is discussed in Appendix B. As usual we restrict the $\vec b^{\,i}$ to be unit vectors. Equation (1) is not the most general form for square lattices and the renormalized parameters have only cubic symmetry in this case, even if we start off with the isotropic model of (1). The discussion here is therefore confined to the triangular lattice.

Since we are primarily interested in large-distance behavior we make a continuum approximation, allowing the vectors to be at any position rather than confined to lattice sites. The underlying lattice only appears through the restriction that no two vectors may be closer than the lattice spacing a_0, which is necessary for stability.[12] We therefore obtain a vector Coulomb gas with a hard-core repulsive interaction at short distances. It is interesting to Fourier transform (1) with the result that

$$H_D = -\frac{\pi}{2}\int d^2q\,\frac{4\pi}{q^2}\left[(K_0^r - K_0^\theta)\,\frac{q_\mu q_\nu}{q^2} + (K_0^r + K_0^\theta)\left(\delta_{\mu\nu} - \frac{q_\mu q_\nu}{q^2}\right)\right] \times b_\mu(q) b_\nu(-q) + \ln y_0 \int d^2q\,\vec{b}(q)\cdot\vec{b}(-q)\,. \tag{48}$$

The dislocation Hamiltonian with $K_0^r = K_0^\theta$ therefore corresponds to a vector Coulomb gas with transverse interaction,[10] whereas if the angular forces are neglected the interaction is equally longitudinal and transverse. For stability both the longitudinal and transverse components must be nonnegative (Halperin, private communication) so the interesting region is $-K_0^r \le K_0^\theta \le K_0^r$, $K_0^r > 0$.

For a given configuration of vector charges we denote the number of these in direction α ($\alpha = 1, \ldots, 6$) by n_α. The partition function may be written

$$Z = \sum_{\{n_\alpha\}} \prod_{\alpha=1}^{6}\left(\frac{1}{n_\alpha!}\right)\int \prod_{i=1}^{N} d^2r^i \left(\frac{y}{a_0^2}\right)^N e^{H(\{n\})}, \tag{49}$$

where

$$N = \sum_{\alpha=1}^{6} n_\alpha \tag{50}$$

and $H(\{n\})$ is the Hamiltonian (1) without the chemical potential term and with a fixed n_α. The region of integration in (49) is over all space except that no two vectors may be closer than a core distance a_0. From now on we drop the subscript 0 on K^r, K^θ, and y and write $H(\{n\})$ as

$$H(\{n\}) = 2\pi \sum_{\langle ij\rangle} b_\mu^i \epsilon_{\mu\alpha} b_\nu^j \epsilon_{\nu\beta} M_{\alpha\beta}(\vec{r}^{ij}), \tag{51}$$

where

$$M_{\alpha\beta}(\vec{r}) = K^r \delta_{\alpha\beta} G(r) + K^\theta (r_\alpha r_\beta / r^2 - \tfrac{1}{2}\delta_{\alpha\beta}). \tag{52}$$

$\epsilon_{\mu\alpha}$ is the usual antisymmetric tensor defined in Appendix A and

$$G(r) = \ln(r/a_0). \tag{53}$$

$M_{\alpha\beta}$ has the following easily verified properties:

$$\partial_\alpha M_{\alpha\beta} = (K^r + K^\theta)\partial_\beta G\,, \tag{54a}$$

$$\epsilon_{\mu\alpha}\partial_\mu M_{\alpha\beta} = (K^r - K^\theta)\partial_\mu G\,\epsilon_{\mu\beta}, \tag{54b}$$

$$\nabla^2 M_{\alpha\beta} = 2\pi(K^r - K^\theta)\delta_{\alpha\beta}\delta(r) + 2K^\theta \partial_\alpha\partial_\beta G, \tag{54c}$$

which will be useful later. In deriving (54c) we have used $\nabla^2 G = 2\pi\delta(r)$.

Consider a pair (i,j) of oppositely oriented vector charges with separation $\vec{r}^{ij}$ such that $a_0 < r^{ij} < a_0' = a_0(1+\delta l)$ with $\delta l \ll 1$. The Hamiltonian for the pair, H_{ij}, consists of a part H_{ij}^0 only involving the pair, given by

$$H_{ij}^0 = \exp(\pi K^\theta \cos 2\theta)\,, \tag{55}$$

where θ is the angle $\vec{r}^{ij}$ makes with the vectors plus a part $\bar{H}_{ij}$, which involves the other dislocations, where

$$\bar{H}_{ij} = 2\pi b_\mu^i \epsilon_{\mu\alpha}\sum_k [M_{\alpha\beta}(\vec{r}^i - \vec{r}^k) - M_{\alpha\beta}(\vec{r}^j - \vec{r}^k)] b_\nu^k \epsilon_{\nu\beta}\,. \tag{56}$$

It is assumed throughout the calculation that y, and hence the mean density of vector charges is small. Consequently it is unlikely that any other charge is within a distance of order a_0 from the pair (i,j). We therefore expand the term in brackets in (56) in powers of a_0/r^{ik} up to quadratic order and find

$$\bar{H}_{ij} = 2\pi b_\mu^i \epsilon_{\mu\alpha}\sum_k [a_\gamma \partial_\gamma M_{\alpha\beta}(\vec{r}^{jk}) + \tfrac{1}{2} a_\gamma a_\eta \partial_\gamma\partial_\eta M_{\alpha\beta}(\vec{r}^{jk})], \tag{57}$$

where we have written a_γ for r_γ^{ij}. Next $e^{\bar{H}_{ij}}$ is expanded in a_0 with the result

$$e^{\bar{H}_{ij}} = 1 + 2\pi b_\mu^i \epsilon_{\mu\alpha}\sum_k [a_\gamma \partial_\gamma M_{\alpha\beta}(\vec{r}^{jk}) + \tfrac{1}{2} a_\gamma a_\eta \partial_\gamma\partial_\eta M_{\alpha\beta}(\vec{r}^{jk})] + 2\pi^2 b_\mu^i \epsilon_{\mu\alpha} b_\rho^i \epsilon_{\nu\beta}\sum_{k,l} a_\gamma \partial_\gamma M_{\alpha\lambda}(\vec{r}^{jk}) \times a_\eta \partial_\eta M_{\beta\pi}(\vec{r}^{jl})\epsilon_{\lambda\rho} b_\rho^k \epsilon_{\pi\chi} b_\chi^l\,. \tag{58}$$

The summation in the last term is an independent summation over all k and all l including terms with $k = l$. One is now in a position to carry out the integration over space in (49) for the pair (i,j). First of all we perform the integral over $\vec{r}^i$, which is an annulus of radius a_0 and thickness $a_0\,dl$ about $\vec{r}^j$ and is denoted by δ_j. The necessary angular averages are easily found to be

$$\langle a_j\rangle = 0\,, \tag{59a}$$

$$\langle a_\gamma a_\eta\rangle = a^2[\tfrac{1}{2}\delta_{\gamma\eta} + (b_\gamma^i b_\eta^i - \tfrac{1}{2}\delta_{\gamma\eta})\langle\cos 2\theta\rangle_{\text{ang}}], \tag{59b}$$

where the average $\langle\cos 2\theta\rangle_{\text{ang}}$ is over the distribution $e^{H_{ij}^0}$ [Eq. (55)] so

$$\langle\cos 2\theta\rangle_{\text{ang}} = I_1(\pi K^\theta)/I_0(\pi K^\theta)\,. \tag{60}$$

From (59) it follows that the second term in (58) is zero. It is also convenient to average over the directions of the pair of vector charges at this stage. Some nonvanishing averages (valid for the triangular but not the square lattice) are given in Appendix A, Eq. (A8), while

$$\langle b_\mu\rangle_{\text{av}} = \langle b_\mu b_\nu b_\alpha\rangle_{\text{av}} = 0\,. \tag{61}$$

From (59b) and (61) we deduce that the third term

in (58) vanishes so we confine our attention to the first and last terms. Equations (55)–(58) now imply that

$$\int_{\delta_j} e^{H_{ij}} = 2\pi a_0^2\, dl\, [I_0(\pi K^\theta) + A_1(\vec{r}^{\,j}) I_0(\pi K^\theta) + A_2(\vec{r}^{\,j}) I_1(\pi K^\theta)], \tag{62}$$

where A_1 and A_2 come from the first and second terms in (59b) and are given by

$$A_1(\vec{r}^{\,j}) = \frac{(\pi a_0)^2}{2} \sum_{k,l} b_\nu^k \epsilon_{\nu\beta} \partial_\eta M_{\alpha\beta}(\vec{r}^{\,jk}) \times b_\lambda^l \epsilon_{\lambda\gamma} \partial_\eta M_{\alpha\gamma}(\vec{r}^{\,jl}), \tag{63a}$$

$$A_2(\vec{r}^{\,j}) = \frac{(\pi a_0)^2}{4} \sum_{k,l} \epsilon_{\mu\alpha} \epsilon_{\nu\beta} b_\rho^k \epsilon_{\rho\lambda} \partial_\gamma M_{\alpha\lambda}(\vec{r}^{\,jk}) \times b_\chi \epsilon_{\chi\pi} \partial_\eta M_{\beta\pi}(\vec{r}^{\,jl}) \times [\delta_{\mu\nu}\delta_{\gamma\eta} + \delta_{\mu\gamma}\delta_{\eta\nu} + \delta_{\mu\eta}\delta_{\gamma\nu}]. \tag{63b}$$

Next we integrate $\vec{r}^{\,j}$ over all space apart from circles of radius a about the remaining $N-2$ vector charges. This region of integration, which is denoted by D_j, actually counts certain configurations which will not occur because $\vec{r}^{\,i}$ will be closer than a to another charge even though $\vec{r}^{\,j}$ is not. Such steric effects are small for pairs (k,l) separated by a distance large compared with a and are irrelevant in the critical region. Integrating (63a) by parts assuming $r^{kl} \gg a_0$, and using (54c) one obtains

$$\int_{D_j} d^2 r_j A_1(\vec{r}_j) = -\frac{(\pi a_0)^2}{2} \left\{ 2\pi (K^r - K^\theta) \sum_{k,l} b_\nu^k \epsilon_{\nu\beta} M_{\alpha\beta}(\vec{r}_{kl}) b_\lambda^l \epsilon_{\lambda\alpha} + 2K^\theta \int_{D_j} d^2 r_j \sum_{k,l} b_\nu^k \epsilon_{\nu\beta} M_{\alpha\beta}(\vec{r}^{\,jk}) \times b_\lambda^l \epsilon_{\lambda\gamma} \partial_\alpha \partial_\gamma G(\vec{r}^{\,jl}) \right\}. \tag{64}$$

The second term in (64) is integrated again by parts and using (54a) together with the result that

$$\int_{D_j} d^2 r_j \sum_{k,l} n_k n_l \partial_\mu G(r^{jk}) \partial_\nu G(r^{jl}) = -2\pi \sum_{\langle k,l \rangle} n_k n_l \left[\delta_{\mu\nu} G(r^{kl}) + \left(\frac{r_\mu^{kl} r_\nu^{kl}}{(r^{kl})^2} - \frac{\delta_{\mu\nu}}{2} \right) \right] \tag{65}$$

valid for $r^{kl} \gg a_0$, $\sum n_k = 0$, we obtain

$$\int_{D_j} d^2 r_j A_1(r_j) = -2\pi^3 a_0^2 \sum_{\langle k,l \rangle} \left[[(K^r)^2 + (K^\theta)^2] \delta_{\alpha\beta} G(r^{kl}) - 2K^r K^\theta \left(\frac{r_\alpha^{kl} r_\beta^{kl}}{(r^{kl})^2} - \frac{\delta_{\alpha\beta}}{2} \right) \right] b_\alpha^k b_\beta^l. \tag{66}$$

The manipulations needed to integrate A_2 over D_j are similar, expect that in addition one needs (54b), and the final result is

$$\int_{D_j} d^2 r_j A_2(r_j) = \pi^3 a_0^2 \sum_{\langle k,l \rangle} \left[2K^r K^\theta \delta_{\alpha\beta} G(r^{kl}) - [(K^r)^2 + (K^\theta)^2] \times \left(\frac{r_\alpha^{kl} r_\beta^{kl}}{(r^{kl})^2} - \frac{\delta_{\alpha\beta}}{2} \right) \right] b_\alpha^k b_\beta^l. \tag{67}$$

We can now collect our results so far into the equation

$$3 \int_{D_j} d^2 r_j \int_{\delta_j} e^{H_{ij}} = \frac{\delta F}{(a_0 y)^2} + \frac{2\pi a_0^4}{y^2} \sum_{\langle k,l \rangle} \left[\delta K^r \delta_{\alpha\beta} G(r^{kl}) - \delta K^\theta \left(\frac{r_\alpha^{kl} r_\beta^{kl}}{(r^{kl})^2} - \frac{\delta_{\alpha\beta}}{2} \right) \right] b_\alpha^k b_\beta^l, \tag{68}$$

where δF, δK^r, and δK^θ are proportional to δl. Since they will eventually appear as an additive contribution to the free energy and the change in K^r and K^θ, respectively, we write $\delta K^r/\delta l$ as dK^r/dl, etc., and obtain the differential equations

$$A^{-1} \frac{dF}{dl} = 6\pi I_0(\pi K^\theta) y^2 \tag{69}$$

and

$$\frac{dK^r}{dl} = -6\pi^3 y^2 \{ [(K^r)^2 + (K^\theta)^2] I_0(\pi K^\theta) - K^r K^\theta I_1(\pi K^\theta) \}, \tag{70a}$$

$$\frac{dK^\theta}{dl} = -6\pi^3 y^2 \{ 2K^r K^\theta I_0(\pi K^\theta) - \tfrac{1}{2} [(K^r)^2 + (K^\theta)^2] I_1(\pi K^\theta) \}, \tag{70b}$$

where A is the area of the system. It is interesting to note that recursion relations for the longitudinal and transverse couplings which from (48) are related to K^r and K^θ by

$$K_L = \tfrac{1}{2}(K^r - K^\theta), \quad K_T = \tfrac{1}{2}(K^r + K^\theta) \tag{71}$$

can be expressed in somewhat simpler form as

$$\frac{dK_L^{-1}}{dl} = 12\pi^3 y^2[I_0(\pi K^\theta) + \tfrac{1}{2} I_1(\pi K^\theta)], \tag{72a}$$

$$\frac{dK_T^{-1}}{dl} = 12\pi^3 y^2[I_0(\pi K^\theta) - \tfrac{1}{2} I_1(\pi K^\theta)]. \tag{72b}$$

The equation for K_T^{-1} is identical to the result obtained for $K^r = K^\theta$, Eq. (25a), with K^θ in the argument of the Bessel functions, while the recursion relations for K_L^{-1} differ only in the sign of the term proportional to I_1 which came from the angular average $\langle \cos 2\theta \rangle_{\text{ang}}$. Comparing with Eq. (16) we see that the longitudinal and transverse polarizabilities of the vector Coulomb gas are given by

$$\alpha_L(r) = \tfrac{1}{2}\pi K_0^L r^2 (1 + \tfrac{1}{2}\langle \cos 2\theta \rangle_{\text{ang}}), \tag{73a}$$

$$\alpha_T(r) = \tfrac{1}{2}\pi K_0^T r^2 (1 - \tfrac{1}{2}\langle \cos 2\theta \rangle_{\text{ang}}). \tag{73b}$$

The analogous result for the scalar Coulomb gas is given by Eq. (9).

The subsequent step is exactly as in Kosterlitz.[2] We have integrated out from the partition function (49) a pair of charges (i, j). The terms in the summation over $\{n_\alpha\}$ are correspondingly rearranged, we allow for the existence of three types of oppositely oriented vector charge, and then we reexponentiate terms of order δl. The result is, as promised, that K^r is replaced by $K^r + \delta K^r$ and K^θ by $K^\theta + \delta K^\theta$.

The hard-core distance a_0 has been increased from a_0 to $a_0(1 + \delta l)$ but the parameter a_0 still appears in the Hamiltonian through (53) and in the expression for the partition function (49). In order to complete the renormalization-group calculation we must replace a_0 by a_0' in these places which is easily shown to generate a change δy_1 in y where

$$\delta y_1 = (2 - \pi K^r)\, y\, \delta l. \tag{74}$$

Since the charges are unit vectors pointing to nearest-neighbor positions on a triangular lattice we must also consider pairs separated by a core distance a_0 whose vectors are not oppositely oriented but the sum of which is another unit vector. These cannot be integrated out because that would violate the charge neutrality condition $\sum_i \vec{b}^i = 0$. Instead we consider them to be a single "composite" charge just as in Sec. II. After rescaling each of the charges can be either one of the original charges or a composite type so we have effectively increased the fugacity y. To leading order in y it follows straightforwardly that the change δy_2 is

$$\delta y_2 = 2\pi I_0(\pi K^\theta)\, y^2\, \delta l. \tag{75}$$

The total change in y is given by the sum $\delta y_1 + \delta y_2$ so we obtain for dy/dl the equation

$$\frac{dy}{dl} = (2 - \pi K^r)\, y + 2\pi I_0(\pi K^\theta)\, y^2. \tag{76}$$

Equations (70) or (72) together with (76) are our final recursion relations. Clearly if $K_0^\theta = 0$ initially then $K^\theta(l) = 0$ at all scales l and similarly if $K_0^r = \pm K_0^\theta$ this equality is preserved by the recursion relations. For $K^r = K^\theta$ we recover the results of the linear-response theory of Sec. II, namely, Eqs. (25a) and (25b), while for $K^\theta = 0$ our equations reduce to Nelson's[9] recursion relations.

The behavior of the solutions to (69) and (73) is largely controlled by the sign of the coefficient of y in (76). If $K^r(l=0)$ is sufficiently large that $K^r(l) > 2/\pi$ for all l then $y \to 0$ and K^θ tends to a constant as $l \to \infty$. If, however, K^r becomes smaller than $2/\pi$ at some l then y diverges as l continues to increase. Consequently there is a fixed surface in the K^r, K^θ plane at $y = 0$, which is stable for $K^r > 2/\pi$ and unstable for $K^r < 2/\pi$. Projected onto the plane $K^\theta = 0$ the trajectories are qualitatively the same as in Fig. 1. The region of stability of the fixed surface terminates in the line $K^r = 2/\pi$ and we shall now show that the exponent $\bar{\nu}$ varies continuously along this line.

To extract the leading temperature dependence of the renormalized couplings we replace K^r and K^θ in the equation for dK^r/dl (70a) by their renormalized values at $T = T_c^-$, namely, $2/\pi$ and $K_R^\theta(T_c^-)$, respectively, and put $K_R^\theta(T_c^-)$ in the argument of the Bessel function in (76). Defining $x = 2 - \pi K^r$ Eqs. (70a) and (76) reduce to the form (28) where

$$\alpha^2 = \tfrac{1}{2} I_0(2\sigma)[1 + \sigma^2 - \sigma I_1(2\sigma)/I_0(2\sigma)]^{-1} \tag{77}$$

with

$$\sigma = K_R^\theta(T_c^-)/K_R^r(T_c^-) = \tfrac{1}{2}\pi K_R^\theta(T_c^-). \tag{78}$$

The interesting region is $-1 < \sigma < 1$ and from (77) α, and hence $\bar{\nu}$, is a symmetric function of σ. The exponent $\bar{\nu}$ is related to α by (43) and a plot of $\bar{\nu}$ against σ for $0 < \sigma < 1$ is shown in Fig. 2. Since α^2 is always rather small the variation in $\bar{\nu}$ is quite modest. For $\sigma \ll 1$ it is straightforward to show that

$$\bar{\nu} = \tfrac{2}{5}(1 - \tfrac{3}{25}\sigma^2 \cdots). \tag{79}$$

K_R^r varies as (42) close to T_c while K_R^θ behaves as

$$K_R^\theta(T) = K_R^\theta(T_c^-) + C' t^{\bar{\nu}},$$

where in general $K_R^\theta(0^-)$ is nonuniversal. As mentioned above, however, $K_R^\theta = 0$ if $K_0^\theta = 0$ while for $K_0^\theta = K_0^r$ we have $K_R^\theta(T_c^-) = 2/\pi$.

One can show by a similar calculation[9] that the correlation ξ_+ varies as

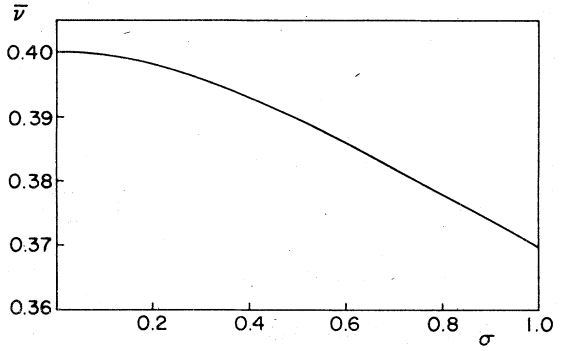

FIG. 2. Plot of the critical exponent $\bar{\nu}$ as a function of σ, the ratio of the renormalized angular to radial interaction at $T = T_c^-$. The radial interaction has the universal value of $2/\pi$ at T_c^-. The curve is derived from Eqs. (43) and (77) of the text which also imply that $\bar{\nu}$ is an even function of σ.

$$\xi_\pm \sim \exp(b_\pm / |t|^{\bar{\nu}}), \tag{80}$$

where $b_\pm$ are nonuniversal. Equation (69) gives an additive contribution to the free energy per unit area from which one can deduce that the singular part, $f_\pm^{\text{sing}}$, has only an essential singularity of the form[2]

$$f_\pm^{\text{sing}} \sim \xi_\pm^{-2}. \tag{81}$$

V. CONCLUSIONS

We have developed the Kosterlitz-Thouless theory of melting on the triangular lattice paying special attention to the angular forces between dislocation pairs. Close to T_c the elastic constants vary as given by Eq. (46) and the exponent $\bar{\nu}$ is calculated to be $0.3696\cdots$, different from the analogous exponent for planar spins and helium films which is $\frac{1}{2}$. This difference arises from an extra term in the recursion relations which in turn is due to the possibility of adding two unit Burger vectors on the triangular lattice to form another unit Burger vector. These results apply to the transition out of the solid phase. As shown by Halperin and Nelson[10] the phase just above T_c is a type of liquid crystal rather than a liquid.

Generalizing the dislocation Hamiltonian to an arbitrary vector Coulomb gas we find that $\bar{\nu}$ changes continuously as one varies the ratio of the renormalized angular to radial interaction at $T = T_c^-$. $\bar{\nu}$ is given explicitly by Eqs. (43) and (77) and is plotted in Fig. 2. Such a model may be appropriate to melting on a periodic substrate[10] but since the change in $\bar{\nu}$ is small the prospects for experimental verification of this nonuniversal behavior seem slight. Although we have not carried out a complete calculation for the square lattice it seems likely that $\bar{\nu} = \frac{1}{2}$ independent of the parameters in the dislocation Hamiltonian.

The crucial assumption in the theory is that the density of dislocations is small at T_c, which may not be true for a realistic solid. Since the density of dislocations decreases upon iterating the recursion relations for $T \leq T_c$ it is possible that our results are correct even for a large initial density. It is also possible, however, that with a large initial density the renormalization-group trajectories flow into another region of the parameter space where the physics is different. Numerical studies should help distinguish between these possibilities.

APPENDIX A

In this Appendix we follow Ref. 10 in developing a linear-response theory for two-dimensional elasticity for the triangular lattice from which we can calculate the reduction of the elastic constants due to screening by dislocation pairs.

Our starting point is the Peach-Koehler[11] formula for the force F_μ on a dislocation due to a uniform external stress $\sigma_{\lambda\nu}$. This states that

$$F_\mu = a_0 b_\lambda \sigma_{\lambda\nu} \epsilon_{\nu\mu}, \tag{A1}$$

where $\epsilon_{\nu\mu}$ is the antisymmetric tensor with nonvanishing elements $\epsilon_{xy} = -\epsilon_{yx} = 1$. The energy E of a pair of oppositely oriented Burger vector separated by $\vec{r}$ due to the stress is obtained by integrating up (A1) so

$$E = a_0 b_\lambda \sigma_{\lambda\nu} \epsilon_{\nu\mu} r_\mu. \tag{A2}$$

This energy must also equal the integral over all space of the stress times the strain[10] so the total strain $U_{\lambda\nu}^{\text{sing}}$ due to the pair is given by

$$U_{\lambda\nu}^{\text{sing}} = \tfrac{1}{2} a_0 (b_\lambda \epsilon_{\nu\mu} r_\mu + b_\nu \epsilon_{\lambda\mu} r_\mu). \tag{A3}$$

[We are grateful to Halperin for an illuminating discussion on this somewhat tricky point. $U_{\lambda\nu}$ is *not* the integral over all space of the local strain $u_{\lambda\nu}(\vec{r})$ because the displacement field is multivalued and so has a cut between the dislocations. One must therefore include the contribution to $U_{\lambda\nu}^{\text{sing}}$ from the discontinuity in the displacement across the cut. A misunderstanding of this point led to an incorrect evaluation of the renormalized elastic constants in a preliminary version of this paper.]

The inverse elastic constant tensor $C_{\gamma\beta\lambda\nu}^{-1}$ can be expressed in terms of the total strain $U_{\lambda\nu}$ as

$$C_{\gamma\beta\lambda\nu}^{-1} = (1/Vk_BT) \langle U_{\gamma\beta} U_{\lambda\nu} \rangle, \tag{A4}$$

where $U_{\lambda\nu}$ is the sum of the total strain due to harmonic lattice vibrations plus the dislocation part which is a sum of terms like (A3) over all pairs. The harmonic contribution gives the bare elastic constants μ_0 and B_0 while the cross term vanishes.[1]

As in the Kosterlitz-Thouless approach it is useful to introduce a scale-dependent elastic constant tensor $C_{\gamma\beta\lambda\nu}(r)$ which includes the screening effect of pairs of separation between a and r. We therefore generalize (A4) to read

$$C^{-1}_{\gamma\beta\lambda\nu}(r)=\frac{1}{4\mu_0}(\delta_{\gamma\lambda}\delta_{\beta\nu}+\delta_{\gamma\nu}\delta_{\beta\lambda}-\delta_{\gamma\beta}\delta_{\lambda\nu})+\frac{1}{4B_0}\delta_{\gamma\beta}\delta_{\lambda\nu}+\frac{a_0^2}{4k_BT}\int_a^r n(r',\theta)\bar{\alpha}_{\gamma\beta\lambda\nu}(r')r'\,dr'\,d\theta\,, \quad \text{(A5)}$$

where $n(r',\theta)$ is the number of pairs of opposite Burger vectors with separation r' whose displacement vector makes an angle θ with one of the Burger vectors. $\bar{\alpha}_{\gamma\beta\lambda\nu}$ is given by

$$\bar{\alpha}_{\gamma\beta\lambda\nu}=\langle\langle(b_\gamma\epsilon_{\beta\mu}r_\mu+b_\beta\epsilon_{\gamma\mu}r_\mu)(b_\lambda\epsilon_{\nu\sigma}r_\sigma+b_\nu\epsilon_{\lambda\sigma}r_\sigma)\rangle\rangle_{\text{ang}}\,, \quad \text{(A6)}$$

where $\langle\cdots\rangle_{\text{ang}}$ devotes an average at fixed r over the distribution arising from the angular interaction between the pair. From Eq. (1) this is $\exp[\pi K(r)\cos2\theta]$, where we have inserted the value of K on the length scale r to include screening of this pair due to smaller pairs. Averaging over the directions of r gives

$$\langle r_\mu r_\sigma\rangle_{\text{ang}}=r^2[\delta_{\mu\sigma}/2+(b_\mu b_\sigma-\tfrac{1}{2}\delta_{\mu\nu})\langle\cos2\theta\rangle_{\text{ang}}]\,. \quad \text{(A7)}$$

It is also convenient to average over directions of the Burger vector $\vec{b}$. On the triangular lattice the only second- and fourth-rank invariant tensors are the same as for an isotropic system so we find

$$\langle b_\mu b_\sigma\rangle_{\text{av}}=\tfrac{1}{2}\delta_{\mu\sigma}\,, \quad \text{(A8a)}$$

$$\langle b_\mu b_\sigma b_\gamma b_\lambda\rangle_{\text{av}}=\tfrac{1}{8}(\delta_{\mu\sigma}\delta_{\gamma\lambda}+\delta_{\mu\gamma}\delta_{\sigma\lambda}+\delta_{\mu\lambda}\delta_{\sigma\gamma})\,. \quad \text{(A8b)}$$

Equation (A8b) is incorrect for the square lattice and the renormalized elastic constant tensor has only cubic symmetry even if we assume the unrenormalized elastic constants have isotropic symmetry. From (A6)–(A8) and the identity $\epsilon_{\mu\sigma}\epsilon_{\gamma\lambda}=\delta_{\mu\gamma}\delta_{\sigma\lambda}-\delta_{\mu\lambda}\delta_{\sigma\gamma}$ it is straightforward to reduce $\bar{\alpha}_{\gamma\beta\lambda\nu}$ to the form

$$\bar{\alpha}_{\gamma\beta\lambda\nu}(r)=\bar{\alpha}_B(r)\delta_{\gamma\beta}\delta_{\lambda\nu}+\bar{\alpha}_\mu(r)(\delta_{\gamma\lambda}\delta_{\beta\nu}+\delta_{\gamma\nu}\delta_{\beta\lambda}-\delta_{\gamma\beta}\delta_{\lambda\nu})\,, \quad \text{(A9)}$$

where

$$\bar{\alpha}_B(r)=\tfrac{1}{2}r^2(1-\langle\cos2\theta\rangle_{\text{ang}})\,, \quad \text{(A10a)}$$

$$\bar{\alpha}_\mu(r)=\tfrac{1}{2}r^2\,. \quad \text{(A10b)}$$

From (A5) and (A9) the scale-dependent elastic constants are given by

$$\mu^{-1}(r)=\mu_0^{-1}+\frac{a_0^2}{k_BT}\int_a^r\bar{\alpha}_\mu(r')n(r',\theta)r'\,dr'\,d\theta\,, \quad \text{(A11a)}$$

$$B^{-1}(r)=B_0^{-1}+\frac{a_0^2}{k_BT}\int_a^r\bar{\alpha}_\beta(r')n(r',\theta)r'\,dr'\,d\theta\,. \quad \text{(A11b)}$$

(A11) together with (2) imply that

$$K^{-1}(r)=K_0^{-1}+2\pi^2\int_a^r[\bar{\alpha}_\mu(r')+\bar{\alpha}_B(r')]\times n(r',\theta)r'\,dr'\,d\theta\,, \quad \text{(A12)}$$

which is equivalent to

$$K(r)=K_0/\epsilon(r)$$

with

$$\epsilon(r)=1+4\pi\int_a^r\alpha(r')n(r',\theta)r'\,dr'\,d\theta\,, \quad \text{(A13)}$$

where the polarizability $\alpha(r')$ is given by

$$\alpha(r')=\tfrac{1}{2}\pi K_0(r')^2(1-\tfrac{1}{2}\langle\cos2\theta\rangle_{\text{ang}})\,. \quad \text{(A14)}$$

Equations (A12) and (A13) are the results used in Sec. II to derive scaling equations for $K(r)$.

APPENDIX B

Nelson and Halperin[10] have discussed the melting of a solid layer on a periodic substrate and concluded that there exist values of the parameters where the substrate applies an orientational bias to the adsorbate but does not give any pinning of the translational degrees of freedom. In this case the solid is described by an elastic Hamiltonian of the form

$$\mathcal{H}_{\text{el}}=\frac{1}{2}\int d^2r\,C^0_{\alpha\beta\gamma\delta}w_{\alpha\beta}(\vec{r})w_{\gamma\delta}(\vec{r})\,, \quad \text{(B1)}$$

where the elastic constant tensor is given by

$$C^0_{\alpha\beta\gamma\delta}=\mu_0(\delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{\alpha\delta}\delta_{\gamma\beta}-\delta_{\alpha\beta}\delta_{\gamma\delta})+B_0\delta_{\alpha\beta}\delta_{\gamma\delta}+\gamma_0\epsilon_{\alpha\beta}\epsilon_{\gamma\delta} \quad \text{(B2)}$$

and the $w_{\alpha\beta}$ are *unsymmetrized* strains defined by

$$w_{\alpha\beta}=\partial_\alpha u_\beta\,, \quad \text{(B3)}$$

where $\vec{u}$ is the displacement field. The substrate appears through the term in (B2) involving γ_0 which is proportional to the square of the local rotation $\theta(\vec{r})$ defined by

$$\theta(\vec{r})=\tfrac{1}{2}[\partial_x u_y(\vec{r})-\partial_y u_x(\vec{r})]\,. \quad \text{(B4)}$$

The dislocation Hamiltonian arising from (B1) has the form given in Eq. (1) but now[10]

$$K_0^r=\frac{1}{2\pi^2}\frac{a_0^2}{k_BT}\left(\frac{\mu_0B_0}{\mu_0+B_0}+\frac{\mu_0\gamma_0}{\mu_0+\gamma_0}\right), \quad \text{(B5a)}$$

$$K_0^\theta=\frac{1}{2\pi^2}\frac{a_0^2}{k_BT}\left(\frac{\mu_0B_0}{\mu_0+B_0}-\frac{\mu_0\gamma_0}{\mu_0-\gamma_0}\right). \quad \text{(B5b)}$$

Denoting the total unsymmetrized strain by $W_{\alpha\beta}$ it follows straightforwardly that the analogs of (A3) and (A4) are

$$W_{\alpha\beta}^{\text{sing}} = a_0 b_\alpha \epsilon_{\beta\lambda} r_\lambda \tag{B6}$$

and

$$C^{-1}_{\alpha\beta\lambda\nu} = \frac{1}{V k_B T} \langle W_{\beta\beta} W_{\lambda\nu} \rangle . \tag{B7}$$

Since the inverse elastic constant tensor must have the form

$$C^{-1}_{\alpha\beta\lambda\nu}(r) = \frac{1}{4\mu(r)} (\delta_{\alpha\lambda}\delta_{\beta\nu} + \delta_{\alpha\nu}\delta_{\beta\lambda} - \delta_{\alpha\beta}\delta_{\lambda\nu}) + \frac{1}{4B(r)} \delta_{\alpha\beta}\delta_{\lambda\nu} + \frac{1}{4\gamma(r)} \epsilon_{\alpha\beta}\epsilon_{\lambda\nu} , \tag{B8}$$

it is easy to project out the parts of (B7) which correspond to the different elastic constants. Proceeding as in Appendix A we find that $\mu^{-1}(r)$ and $B^{-1}(r)$ are still given by (A11) with the same $\bar{\alpha}_B(r)$ and $\bar{\alpha}_\mu(r)$, while $\gamma^{-1}(r)$ has an analogous expression but with

$$\bar{\alpha}_\gamma(r) = \tfrac{1}{2} r^2 (1 + \langle \cos 2\theta \rangle_{\text{ang}}) . \tag{B9}$$

The recursion relations for μ and B are therefore still given by Eq. (45) (with K^θ in the argument of the Bessel functions) and the corresponding equation for γ is

$$\frac{k_B T}{a_0^2} \frac{d\gamma^{-1}}{dl} = 3\pi y^2 [I_0(\pi K^\theta) + I_1(\pi K^\theta)] . \tag{B10}$$

It is now straightforward to show that Eqs. (45), (B5), and (B10) are equivalent to Eqs. (71) and (72).

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