

## Study of melting in two dimensions

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Techniques developed in studies of the two-dimensional planar model of magnetism are applied to the Kosterlitz-Thouless dislocation model of melting in two dimensions. Duality transformations relate the dislocation problem to Hamiltonians with short-ranged interactions amenable to a Migdal-Kadanoff recursion-relation analysis. In an approximation which neglects an angular dependence in the decay of correlations, the melting problem is equivalent to the statistical mechanics of two interpenetrating superfluids with coupled phases. The coupling between the phases is a marginal operator which (together with other marginal couplings) destroys the universality of critical exponents at the melting temperature  $T_m$ . Indeed melting seems to bear roughly the same relation to the planar model as the Baxter model does to the Ising model. A recursion scheme similar to that developed by Kosterlitz for the planar model is used to study the correlation length, specific heat, and Burger's-vector correlations near melting. For melting of a triangular lattice, the correlation length diverges,  $\xi_+ \sim \exp[C(T/T_m - 1)^{-2/5}]$ , as  $T$  approaches  $T_m$  from above. There is an analogous essential singularity in the specific heat.

### I. INTRODUCTION

The statistical mechanics of systems with a continuous symmetry in two dimensions is especially peculiar. High-temperature series expansions for classical spins with a continuous rotational symmetry<sup>1-4</sup> suggest a finite-temperature phase transition, despite rigorous proofs of the absence of conventional long-range order<sup>5-7</sup> in such systems. Spin-wave calculations by Wegner<sup>8</sup> and Berezinskii<sup>9</sup> indicate the existence, for  $n=2$  component spins, of a bizarre low-temperature phase in which correlations decay as power laws with temperature-dependent exponents. Kane and Kadanoff<sup>10</sup> have arrived at similar conclusions for two-dimensional superfluids.

A two-dimensional solid, where the important symmetry is translational rather than rotational, has some similarity to superfluids and planar (or two-component) models of magnetism in  $d=2$ . Despite arguments due to Peierls<sup>11</sup> and Landau<sup>12</sup> (and a rigorous proof by Mermin<sup>13</sup>) that ordinary long-range order cannot exist in such systems, Janocovici<sup>14</sup> has shown that a theory of harmonic phonons gives rise to a low-temperature "crystalline" phase with  $\delta$ -function Bragg peaks in the structure factor replaced by temperature-dependent power-law singularities.

Kosterlitz and Thouless<sup>15</sup> have proposed that transitions out of such anomalous low-temperature phases are driven by the dissociation of bound pairs of singularities. In a lattice of two-component spins, bound vortex-antivortex pairs populate a low-temperature phase, coexisting with spin-wave excitations. The dissociation of these pairs above a critical temperature  $T_c$  gives rise to an exponential decay of correlations

at high temperatures. Bound dislocation pairs (with equal and opposite Burger's vectors) are presumed to play a similar role in two-dimensional crystals,<sup>15</sup> coexisting with phonons at low temperatures. Although Berezinskii<sup>16</sup> has advanced similar ideas for spin systems and crystals, he failed to distinguish between  $n=2$  and  $n=3$  component spins. Recent work on phase transitions in  $2+\epsilon$  dimensions<sup>17-20</sup> strongly suggests that spin models with  $n \geq 3$  components have no finite-temperature phase transition in  $d=2$ . According to reports by Elgin and Goodstein,<sup>21</sup> Feynman has also viewed the problem of melting in two dimensions in terms of the dissociation of dislocation pairs. The predictions of a harmonic theory of phonons have been worked out in detail by Imry and Gunther,<sup>22</sup> who also discuss effects due to the finite size of the sample.

Kosterlitz,<sup>23</sup> and subsequently José *et al.*,<sup>24</sup> have produced quantitative model calculations which make the vortex pair picture of magnetic phase transitions in two dimensions concrete. Duality transformations and an approximate recursion-relation analysis were used in Ref. 24 to argue that the detailed predictions that Kosterlitz obtained for a particular model were in fact *universal* for  $d=2$  magnets with an underlying XY symmetry. The theories of Refs. 23 and 24 predict a universal jump in the superfluid density of two-dimensional superfluids,<sup>25</sup> which should ultimately allow a precision experimental test of their validity.

In this paper, we undertake a detailed study of melting in two dimensions, based on the Kosterlitz-Thouless ideas<sup>15</sup> and building on calculational techniques developed by Kosterlitz<sup>23</sup> and by José *et al.*<sup>24</sup> We first relate an effective Hamiltonian

with logarithmically interacting dislocations to a statistical-mechanical problem with short-ranged interactions, in order to better study the universality of this description of interacting singularities. The resulting local problem is easily treated using a bond-moving recursion-relation scheme developed by Migdal<sup>18</sup> and by Kadanoff.<sup>26</sup> In an approximation which neglects an angular dependence in the decay of correlations, we find that the melting problem is equivalent to the statistical mechanics of two interpenetrating superfluids with coupled phases. The Hamiltonians we have studied appear to relax after several iterations of a renormalization-group transformation to a *surface* of fixed points parametrized by an effective temperature and the strength of the coupling between the superfluids. The fixed-point Hamiltonians obtained in this way confirm the universality of an effective Hamiltonian with logarithmically interacting dislocations. This local representation of the melting problem can be exploited to show analytically the existence of several marginal operators, and the irrelevancy of dislocation excitations with large Burger's vectors.

Armed with an understanding of the stability (in the sense of renormalization theory) of this simple model of melting, we carry out a detailed scaling analysis of the effect of dislocation pairs similar to that undertaken by Kosterlitz<sup>23</sup> and by José *et al.*<sup>24</sup> for planar spins. The results are qualitatively similar to those for magnetic systems, as has been suggested previously by Kosterlitz and Thouless.<sup>27</sup> In particular, we find an exponentially diverging correlation length above and below  $T_c$ , and an essential singularity in the specific heat at  $T_m$ . In contrast to the results for two-component magnets, the presence of several marginal operators destroys the universality of the critical behavior at the melting temperature. In fact, melting bears qualitatively the same relation to the planar model as the Baxter model does to the Ising model in two dimensions. Below  $T_m$ , the long-wavelength properties of the crystal can be described entirely in terms of a harmonic Hamiltonian with no dislocations, provided one uses renormalized Lamé coefficients  $\mu_R$  and  $\lambda_R$ . The renormalization of  $\mu_R$  and  $\lambda_R$  near melting, as well as the effect of weak periodic substrate potential on the results presented here, will be discussed in a subsequent publication.<sup>28</sup>

The organization of this paper is as follows: In Sec. II, we discuss an effective Hamiltonian for dislocations. Various duality transformations which allow the global universality of this description to be studied analytically and through the use of approximate recursion relations are discussed in Sec. III. In Sec. IV, the scaling

equations for dislocations are calculated and the properties of crystal near its melting temperature are determined. Various singularities which occur at the melting transition are discussed in Sec. V. Issues which must be resolved before the Kosterlitz-Thouless model of dislocation-mediated melting can be applied to real physical systems (such as adsorbed monolayer films) are discussed in Sec. VI.

## II. HARMONIC PHONONS AND DISLOCATION HAMILTONIAN

One conclusion of this paper is that a simple theory of harmonic phonons such as that discussed by Jancovici<sup>14</sup> becomes an arbitrarily accurate description of the long-wavelength properties of two-dimensional crystals below the melting temperature.<sup>29</sup> The harmonic prediction for the structure factor near a Bragg point, for example, is correct provided one uses elastic constants normalized by the effect of dislocations.<sup>28</sup> In this section, we discuss a continuum description of harmonic phonons, modified by the presence of dislocation singularities in the phonon field, a description due originally to Kosterlitz and Thouless.<sup>15, 27</sup>

Consider the reduced Hamiltonian which arises in standard treatments of continuum elasticity theory,<sup>30</sup>

$$\bar{\mathcal{C}} \equiv -\frac{H}{k_B T} = -\frac{1}{2} \int \frac{d^2 r}{a_0^2} \left( 2\bar{\mu} u_{ij}^2 + \bar{\lambda} u_{kk}^2 \right), \quad (2.1)$$

where  $\bar{\mu}$  and  $\bar{\lambda}$  are the usual elastic constants divided by  $k_B T$  and multiplied by the squared lattice spacing  $a_0$  of the underlying lattice,

$$\bar{\mu} \equiv \mu a_0^2 / k_B T, \quad \bar{\lambda} \equiv \lambda a_0^2 / k_B T, \quad (2.2)$$

and  $u_{ij}(\vec{r})$  is the strain tensor corresponding to a displacement field  $\vec{u}(\vec{r})$ ,

$$u_{ij}(\vec{r}) = \frac{1}{2} \left( \frac{\partial u_i(\vec{r})}{\partial r_j} + \frac{\partial u_j(\vec{r})}{\partial r_i} \right). \quad (2.3)$$

Assuming that the medium is subject to periodic boundary conditions, it is often convenient to integrate (2.1) by parts and obtain an equivalent description in terms of the displacements,

$$\bar{\mathcal{C}} = -\frac{1}{2} \int \frac{d^2 r}{a_0^2} \left[ \bar{\mu} (\vec{\nabla} \cdot \vec{u})^2 + (\bar{\mu} + \bar{\lambda}) (\vec{\nabla} \cdot \vec{u})^2 \right]. \quad (2.4)$$

Equilibrium averages can be calculated with (2.4) by integrating over all configurations of the displacement field  $\vec{u}(\vec{r})$ , provided we imposed a short-distance cutoff which simulates the effect of an underlying lattice.

Kosterlitz and Thouless<sup>15, 27</sup> have emphasized that the translational and rotational symmetries

of such a lattice can give rise to important singularities in the displacement field. Dislocations in particular, as opposed to higher-energy excitations such as disclinations, are assumed to be responsible for melting in two dimensions. A dislocation at the point  $\vec{r}$  can be characterized by the amount by which a contour taken around  $\vec{r}$  fails to close,

$$\oint d\vec{u} = a_0 \vec{b}(\vec{r}), \quad (2.5)$$

where  $\vec{b}(\vec{r}) = n(\vec{r})\vec{e}_1 + m(\vec{r})\vec{e}_2$  is the (dimensionless) Burger's vector<sup>31, 32</sup> of the singularity. Here,  $n(\vec{r})$  and  $m(\vec{r})$  are integers,  $a_0$  is the lattice spacing, and  $a_0\vec{e}_2$  are the basis vectors of the underlying Bravais lattice.

We shall be primarily interested in melting of triangular lattices, which are the most close-packed periodic structures in two dimensions. Both triangular and hexagonal lattices can be described in the harmonic approximation by an isotropic Hamiltonian of the form (2.1).<sup>30</sup> The Burger's vectors of dislocations on a hexagonal lattice with spacing  $a_0$  form a triangular array with spacing  $\sqrt{3}a_0$ . Provided disclinations can be neglected, we expect that melting of a hexagonal crystal will be described by the theory appropriate for a triangular lattice. In addition to a triangular array, we shall also consider melting of a square lattice, described in the harmonic approximation by (2.1). Although this model is somewhat artificial, since in reality *three* elastic constants are necessary to describe a square-lattice crystal,<sup>30</sup> its treatment is somewhat simpler than for a triangular array.

To display explicitly the effect of dislocations on (2.1), we write

$$u_{ij}(\vec{r}) = \phi_{ij}(\vec{r}) + u_{ij}^{\text{sing}}(\vec{r}), \quad (2.6)$$

where  $\phi_{ij}(\vec{r}) \equiv \frac{1}{2}(\partial_i\phi_j + \partial_j\phi_i)$  is the stress tensor associated with a set of smoothly varying displacements  $\vec{\phi}(\vec{r})$ , and  $u_{ij}^{\text{sing}}(\vec{r})$  is the contribution from a collection of dislocation singularities represented by the field  $\vec{b}(\vec{r})$ . According to Refs. 31 and 32,  $u_{ij}^{\text{sing}}(\vec{r})$  can be conveniently expressed in terms of the singular part of the stress tensor  $p_{ij}(\vec{r})$ ,

$$u_{ij}^{\text{sing}} = (1/2\mu)p_{ij}^{\text{sing}} - [\lambda/4\mu(\lambda + \mu)]p_{kk}^{\text{sing}}\delta_{ij}, \quad (2.7)$$

which itself may be written in terms of scalar function  $\chi(r)$ ,<sup>33</sup>

$$\overline{\mathcal{K}}_D = \frac{Ka_0^2}{8\pi k_B T} \int \frac{d^2r}{a^2} \int_{|\vec{r}-\vec{r}'|>a} \frac{d^2r'}{a^2} \left[ \vec{b}(\vec{r}) \cdot \vec{b}(\vec{r}') \ln \left( \frac{|\vec{r}-\vec{r}'|}{a} \right) - \frac{\vec{b}(\vec{r}) \cdot (\vec{r}-\vec{r}') \vec{b}(\vec{r}') \cdot (\vec{r}-\vec{r}')}{|\vec{r}-\vec{r}'|^2} + \vec{b}(\vec{r}) \cdot \vec{b}(\vec{r}') (C+1) \right], \quad (2.17)$$

$$p_{ij}^{\text{sing}} = \epsilon_{ik} \epsilon_{jl} \partial_k \partial_l \chi(\vec{r}). \quad (2.8)$$

The function  $\chi(r)$  obeys the equation<sup>31, 32</sup>

$$\nabla^4 \chi(r) = Ka_0 \int \frac{d^2r'}{a^2} \epsilon_{ij} \frac{\partial}{\partial r_i} [b_j(\vec{r}') \delta(\vec{r}-\vec{r}')], \quad (2.9)$$

whose solution may be written

$$\chi(r) = a_0 \int \frac{d^2r'}{a^2} b_i(\vec{r}') \tilde{G}_i(\vec{r}-\vec{r}'), \quad (2.10)$$

where

$$K = 4\mu(\mu + \lambda)/(2\mu + \lambda). \quad (2.11)$$

The quantity  $\tilde{G}_i(\vec{r}-\vec{r}')$ , which is closely related to the Green's function of (2.9), satisfies the periodic boundary conditions, and is given approximately by

$$\tilde{G}_i(\vec{r}) = -\frac{K}{4\pi} \epsilon_{ij} r_j \left[ \ln \left( \frac{r}{a} \right) + C \right] \quad (2.12)$$

for  $\vec{r}$  large and far from the boundaries. The number  $a$  is a short-distance cutoff or "core diameter" for the dislocation, while  $C$  is a positive constant whose value depends on the lattice structure. The core diameter  $a$  need not be the same as the lattice spacing  $a_0$ .

On inserting (2.6) into (2.1), and making use of (2.7) and (2.8), the Hamiltonian breaks into two parts,

$$\overline{\mathcal{H}} = \overline{\mathcal{H}}_0 + \overline{\mathcal{H}}_D, \quad (2.13)$$

where

$$\overline{\mathcal{H}}_0 = -\frac{1}{2} \int \frac{d^2r}{a^2} [\bar{\mu}(\vec{\nabla} \cdot \vec{\phi})^2 + (\bar{\mu} + \bar{\lambda})(\vec{\nabla} \cdot \vec{\phi})^2] \quad (2.14)$$

is the purely harmonic contribution, and the effect of dislocations is given by

$$\overline{\mathcal{H}}_D = -\frac{1}{\mu k_B T} \int \frac{d^2r}{a^2} \left[ \left( \frac{\partial^2 \chi(r)}{\partial r_i \partial r_j} \right)^2 - \left( \frac{\lambda}{2(\mu + \lambda)} \right) [\nabla^2 \chi(r)]^2 \right]. \quad (2.15)$$

We can evaluate  $\overline{\mathcal{H}}_D$  by first integrating by parts,

$$\overline{\mathcal{H}}_D = -\frac{1}{K k_B T} \int \frac{d^2r}{a^2} \chi(r) \nabla^4 \chi(r), \quad (2.16)$$

and by then making use of (2.9), (2.10), and (2.12) to obtain

where we have excluded configurations in which two dislocations approach each other at distances closer than the core diameter  $a$ . In deriving (2.17), we have made use of the identity, valid for any  $\vec{R}$ ,  $\vec{b}(\vec{r})$ , and  $\vec{b}(\vec{r}')$ ,

$$b_i(\vec{r})\epsilon_{ij}R_j b_m(\vec{r}')\epsilon_{mn}R_n + b_i(\vec{r})R_i b_j(\vec{r}')R_j = b_i(\vec{r})b_i(\vec{r}')R^2. \quad (2.18)$$

Equation (2.17) gives the energy for only those complexions of Burger's vectors with

$$\int d^2r \vec{b}(\vec{r}) = 0. \quad (2.19)$$

There is an infinite energy (in the limit of infinite volume), associated with configurations that do not satisfy this vector "charge conservation"

$$\overline{\mathcal{H}}_D = \frac{\bar{K}}{8\pi} \int \frac{d^2r}{a^2} \int_{|\vec{r}-\vec{r}'|>a} \frac{d^2r'}{a^2} \left[ \vec{b}(\vec{r}) \cdot \vec{b}(\vec{r}') \ln \left( \frac{|\vec{r}-\vec{r}'|}{a} \right) - \frac{\vec{b}(\vec{r}) \cdot (\vec{r}-\vec{r}') \vec{b}(\vec{r}') \cdot (\vec{r}-\vec{r}')}{|\vec{r}-\vec{r}'|^2} \right] + \ln(y) \int \frac{d^2r}{a^2} b^2(\vec{r}), \quad (2.21)$$

where

$$\bar{K} = K a_0^2 / k_B T, \quad y = \exp[-(C+1)\bar{K}/8\pi]. \quad (2.22)$$

Note that  $y$  becomes exponentially small as  $T \rightarrow 0$ .

To calculate the average of any quantity in the ensemble specified by (2.13), we must integrate over smoothly varying displacements  $\vec{\phi}(\vec{r})$  and over distinct complexions of Burger's vectors specified by  $\vec{b}(\vec{r})$ . At low temperatures, we expect that  $\vec{b}(\vec{r})$  will be zero nearly everywhere, and equal to  $\pm \vec{e}_1$ ,  $\pm \vec{e}_2$ , and  $\pm \vec{e}_1 \pm \vec{e}_2$  at isolated points. Although it appears from (2.13), (2.14), and (2.21) that the harmonic excitations in  $\overline{\mathcal{H}}_0$  are decoupled from the dislocations in  $\overline{\mathcal{H}}_D$ , most correlation functions depend on both the phonon and dislocation degrees of freedom. The effect of the dislocation field on such correlation functions can be absorbed into renormalizations of the elastic constants  $\bar{\mu}$  and  $\bar{\lambda}$  which enter (2.14).<sup>28</sup> In the present paper, however, we will concentrate on the statistical mechanics associated with the dislocation degrees of freedom.

$$\Gamma_B(\vec{r}) = -2y^2(r/a)^{-\bar{K}/4\pi} \left\{ \exp[-(\bar{K}/4\pi) \cos^2\theta] + \exp[-(\bar{K}/4\pi) \cos^2(\theta + 2\pi/3)] + \exp[-(\bar{K}/4\pi) \cos^2(\theta - 2\pi/3)] \right\} + O(y^3) \quad (3.2)$$

when the excitations form a triangular lattice. The angle  $\theta$  entering (3.1) and (3.2) is the angle between  $\vec{e}_1$  or  $\vec{e}_2$  and the separation vector  $\vec{r}$ . We expect that (3.1) and (3.2) provide an accurate

condition. This constraint can be used to simplify a portion of (2.17):

$$(C+1) \frac{K a_0^2}{8\pi k_B T} \int \int_{|\vec{r}-\vec{r}'|>a} \frac{dr}{a} \frac{dr'}{a} b(r) \cdot b(r') = -(C+1) \frac{K a_0^2}{8\pi k_B T} \times \int \int_{|\vec{r}-\vec{r}'|<a} \frac{d^2r}{a^2} \frac{d^2r'}{a^2} \vec{b}(\vec{r}) \cdot \vec{b}(\vec{r}') \approx -(C+1) \frac{K a_0^2}{8\pi k_B T} \int \frac{d^2r}{a^2} b^2(r). \quad (2.20)$$

In its final form, the Hamiltonian for dislocations is thus

### III. DUALITY TRANSFORMATIONS AND APPROXIMATE RECURSION RELATIONS

#### A. Angular terms in the dislocation Hamiltonian

Provided the dot product or angular terms in (2.21) can be neglected, the dislocation Hamiltonian  $\overline{\mathcal{H}}_D$  is just a vector generalization of the Coulomb gas which arises in studies of magnets and superfluids.<sup>15, 23-25</sup> To see the effect of the angular part of  $\overline{\mathcal{H}}_D$ , consider the correlations between two Burger's vectors at large separations  $\vec{r}$ . To leading order  $y$ , we have

$$\Gamma_B(\vec{r}) \equiv \langle \vec{b}(\vec{0}) \cdot \vec{b}(\vec{r}) \rangle = -2y^2(r/a)^{-\bar{K}/4\pi} \times \left\{ \exp[-(\bar{K}/4\pi) \cos^2\theta] + \exp[-(\bar{K}/4\pi) \sin^2\theta] \right\} + O(y^4) \quad (3.1)$$

when the allowed Burger's vectors form a square lattice, and

representation of the decay at low temperatures, since  $y$  becomes exponentially small with decreasing  $T$ . As will become evident in Sec. IV, the large- $r$  behavior of  $\Gamma_B(r)$  and of related cor-

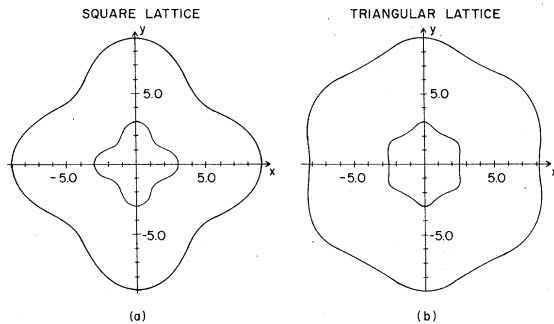


FIG. 1. Contours of constant correlation between Burger's vectors for melting of (a) square and (b) triangular lattices. The correlation  $\Gamma_B(\vec{r})$  is normalized to unity at nearest-neighbor separations, and the contours shown satisfy the condition  $\Gamma_B(\vec{r}) \approx -0.0002$ . The outer "surfaces" of constant correlation are for  $\bar{K} = 16\pi$ , which is very close to the melting temperature. The inner "surfaces" correspond to a lower temperature,  $\bar{K} = 32\pi$ .

relations between Burger's vectors controls the dislocation unbinding at the melting temperature.

Surfaces of constant correlation for the square and triangular lattices are displayed in Fig. 1. Although the angular part of  $\bar{\mathcal{C}}_D$  is numerically negligible compared to the logarithm at large  $\vec{r}$ , it does give rise to a characteristic angular dependence of  $\Gamma_B(\vec{r})$  that persists indefinitely. Apparently, correlations "remember" the orientation of the underlying lattice, which is consistent with Mermin's observation<sup>13</sup> that two-dimensional harmonic solids display long-range "orientational order." A measure of the anisotropy in such correlations is the ratio of the maximum to the minimum radius vector on a surface of constant correlation. For a square lattice, this ratio varies monotonically from 1.65 at low temperatures to about 1.4 near melting (as we shall see, melting occurs when  $\bar{K} \approx 16\pi$ ). For a triangular lattice, the variation is from 1.3 to 1.1.

In Appendix A, we demonstrate that the angular part of  $\bar{\mathcal{C}}_D$  represents, in the jargon of renormalization theory, a *marginal* perturbation to the Coulomb gas obtained by neglecting it. Marginal operators which lead to an angular dependence in the falloff of correlations often arise in studies of critical phenomena. For example, one expects that an Ising model with different nearest-neighbor couplings in the  $x$ ,  $y$ , and  $z$  directions will have ellipsoidal surfaces of constant correlation.<sup>34</sup> Although the operator corresponding to this spatial anisotropy is marginal, it does not change the Ising-model critical exponents. The angular terms in  $\bar{\mathcal{C}}_D$  also resemble a "pseudodipolar"<sup>35</sup> coupling

of nearest-neighbor vector spins studied by Fisher and Aharony.<sup>36</sup> A second order in  $\epsilon$  ( $\epsilon = 4 - d$ ) calculation<sup>37</sup> eventually showed that such perturbations are irrelevant to critical behavior in magnets.

Because a detailed treatment of the angular part of (2.21) presents technical difficulties near the melting temperature, we shall attempt to approximate its effect by replacing it by an angular average. This amounts to substituting circles for the contours in Fig. 1. The vector Coulomb problem which remains is still rather complicated, and in fact exhibits the qualitative behavior one expects for a dislocation-mediated melting transition. We indicate how the complete dislocation Hamiltonian (2.21) could be studied using a Migdal-Kadanoff recursion scheme in Appendix A.

### B. Local formulation of the dislocation problem

Motivated by the discussion in Sec. III B, we consider a simplified version of  $\bar{\mathcal{C}}_D$  with only a Coulomb interaction between vortices, namely,

$$\begin{aligned} \bar{\mathcal{C}}_C = & \frac{\bar{K}}{8\pi} \int \frac{d^2r}{a^2} \int_{|\vec{r}-\vec{r}'|>a} \frac{d^2r'}{a^2} \vec{b}(\vec{r}) \cdot \vec{b}(\vec{r}') \\ & \times \ln(|\vec{r}-\vec{r}'|/a) \\ & + \ln(\bar{y}) \int \frac{d^2r}{a^2} b^2(\vec{r}). \end{aligned} \quad (3.3)$$

The parameter  $\bar{y}$  now includes a contribution from averaging the angular part of (2.21) over orientations of the separation vector  $\vec{r}-\vec{r}'$  in the most likely excited state at low temperatures—two dislocations at  $\vec{r}$  and  $\vec{r}'$  with  $\vec{b}(\vec{r}) = -\vec{b}(\vec{r}')$ . Estimating  $\bar{y}$  in this way, we find

$$\bar{y} \approx \exp[-(C + \frac{3}{2})\bar{K}/8\pi], \quad (3.4)$$

where the  $\frac{3}{2}$  in the exponent comes from the angular average of  $\cos^2\theta$ . Of course, one can imagine other ways of eliminating the angular dependence of  $\bar{\mathcal{C}}_D$ . The physics at the melting transition turns out to be independent of precise value of  $\bar{y}$ , however.

José *et al.*<sup>24</sup> have shown that a scalar Coulomb gas similar to (3.3) arises from a series of duality transformations applied to two-component spins on a lattice. At an intermediate stage in this analysis, one obtains a local formulation of the Coulomb problem which allows an immediate assessment of the stability of this description to small perturbations. We have found it convenient to work backwards from (3.3), and obtain the corresponding local description of melting.

Let  $Z_C$  be the partition function obtained from (3.3) by integrating over Burger's vectors,

$$Z_c = \sum'_{\{\vec{b}(\vec{r})\}} e^{\mathcal{H}_c}, \quad (3.5)$$

where the prime restricts the sum to configura-

tions consistent with vector charge neutrality. The statistical mechanics associated with (3.6) is, in fact, closely related to that determined by the partition sum

$$Z'_c = \sum_{\{p(\vec{r})=-\infty\}} \sum_{\{q(\vec{r})=-\infty\}} \left[ \exp\left(-\frac{4\pi^2}{K(1-x^2)}\right) \sum_{\langle\vec{r},\vec{r}'\rangle} \{[p(\vec{r})-p(\vec{r}')]^2 + [q(\vec{r})-q(\vec{r}')]^2 - 2x[p(\vec{r})-p(\vec{r}')] \times [q(\vec{r})-q(\vec{r}')]\} \right], \quad (3.6)$$

where  $p(\vec{r})$  and  $q(\vec{r})$  are integer-valued variables defined on the sites  $\vec{r}$  of a square lattice, and  $x$  is the inner product of the basis vectors of the Burger's lattice,

$$x = \vec{e}_1 \cdot \vec{e}_2. \quad (3.7)$$

The square lattice on which we have placed the  $p$ 's and  $q$ 's has absolutely no relation to the lattice of allowed Burger's vectors. It merely provides an explicit ultraviolet cutoff, and fits naturally into the duality arguments and recursion-relation analysis of Sec. III C. The summation over  $\vec{r}$  and  $\vec{r}'$  in (3.6) is restricted to nearest-neighbor pairs, so this description is indeed a local one.

To see that  $Z'_c$  is really  $Z_c$  in disguise, we apply the Poisson summation formula<sup>38</sup> to the sums over  $p$  and  $q$ ,

$$Z'_c = \sum_{\{n(\vec{r})=-\infty\}} \sum_{\{m(\vec{r})=-\infty\}} \left( \prod_{\vec{r}} \int_{-\infty}^{\infty} dP(\vec{r}) \right) \left( \prod_{\vec{r}} \int_{-\infty}^{\infty} dQ(\vec{r}) \right) \times \left( \exp - \frac{4\pi^2}{K(1-x^2)} \sum_{\langle\vec{r},\vec{r}'\rangle} \{[P(\vec{r})-P(\vec{r}')]^2 + [Q(\vec{r})-Q(\vec{r}')]^2 - 2x[P(\vec{r})-P(\vec{r}')][Q(\vec{r})-Q(\vec{r}')]\} + 2\pi i \sum_{\vec{r}} [m(\vec{r})P(\vec{r}) + n(\vec{r})Q(\vec{r})] \right), \quad (3.8)$$

and then diagonalize the quadratic form in  $P$  and  $Q$ . On defining

$$\vec{\phi}(\vec{r}) \equiv \frac{P(\vec{r}) - xQ(\vec{r})}{1-x^2} \vec{e}_1 + \frac{P(\vec{r}) + xQ(\vec{r})}{1-x^2} \vec{e}_2, \quad (3.9)$$

we find that Eq. (3.8) can be rewritten rather compactly,

$$Z'_c = \sum_{\{\vec{b}(\vec{r})\}} \int \mathcal{D}\vec{\phi} \exp\left(-\frac{4\pi^2}{K} \sum_{\langle\vec{r},\vec{r}'\rangle} [\vec{\phi}(\vec{r}) - \vec{\phi}(\vec{r}')]^2 + 2\pi i \sum_{\vec{r}} \vec{b}(\vec{r}) \cdot \vec{\phi}(\vec{r})\right), \quad (3.10a)$$

where  $\int \mathcal{D}\vec{\phi}$  means a functional integral over  $\vec{\phi}(\vec{r})$ , and

$$\vec{b}(\vec{r}) = m(\vec{r}) \vec{e}_1 + n(\vec{r}) \vec{e}_2. \quad (3.10b)$$

Carrying out the Gaussian integrations over  $\vec{\phi}(\vec{r})$ , we are led immediately to a quantity proportional to the vector Coulomb-gas partition sum (3.6) (see Appendix A), with, however,

$$\bar{y} \approx e^{-\bar{K}/16} \quad (3.11)$$

replacing Eq. (3.4). The charge-conservation condition arises as a byproduct of the functional integration, and we must make use of an approximate long-wavelength form of the Green's function for a square lattice. This local representation of the dislocation partition function becomes especially useful when we consider finally a generalization of (3.10), namely,

$$Z'_c = \sum_{\{\vec{b}(\vec{r})\}} \int \mathcal{D}\vec{\phi} \exp\left\{-\frac{4\pi^2}{K} \sum_{\langle\vec{r},\vec{r}'\rangle} [\vec{\phi}(\vec{r}) - \vec{\phi}(\vec{r}')]^2 + \sum_{\vec{r}} [\ln y_0 b^2(\vec{r}) + 2\pi i \vec{b}(\vec{r}) \cdot \vec{\phi}(\vec{r})]\right\}, \quad (3.12)$$

so that (3.11) becomes

$$y \approx y_0 e^{-\bar{K}/16}. \quad (3.13)$$

The new parameter  $\ln y_0$  can be interpreted as a core energy associated with each dislocation. Even if  $\ln y_0 = 0$  initially, a nonzero value of  $y_0$  is generated after one iteration of the renormalization transformation described in Sec. IV. Although  $y_0$  could be adjusted to force (3.13) to agree

with (3.4), the renormalization equations constructed in Sec. IV actually drive  $y_0$  to zero below the melting temperature. Dislocations then occur with small probability, and their effect on the Gaussian or "harmonic" part of (3.12) can be treated perturbatively. In this limit, we can carry out the summations over Burger's vectors in (3.12). For a triangular lattice, we find

$$\sum_{\vec{b}(\vec{r})} \exp [\ln(y_0) b^2(\vec{r}) + 2\pi i \vec{b}(\vec{r}) \cdot \vec{\phi}(\vec{r})] = 1 + 2y_0 \cos(2\pi \vec{e}_a \cdot \vec{\phi}) + 2y_0 \cos(2\pi \vec{e}_b \cdot \vec{\phi}) + 2y_0 \cos(2\pi \vec{e}_c \cdot \vec{\phi}) + O(y_0^3) \\ \approx \exp \{ 2y_0 [\cos(2\pi \vec{e}_a \cdot \vec{\phi}) + \cos(2\pi \vec{e}_b \cdot \vec{\phi}) + \cos(2\pi \vec{e}_c \cdot \vec{\phi})] \}, \quad (3.14)$$

where

$$\vec{e}_a = (1, 0), \quad \vec{e}_b = (-\frac{1}{2}, \frac{1}{2}\sqrt{3}), \quad \vec{e}_c = (-\frac{1}{2}, -\frac{1}{2}\sqrt{3}), \quad (3.15)$$

with a similar result for other lattices. Hence, (3.12) is equivalent for a triangular lattice of Burger's vectors and for small  $y_0$  to a vector version of a sine-Gordon<sup>39</sup> partition sum, namely,

$$Z'_c \approx \int \mathcal{D} \vec{\phi} \exp \left( -\frac{4\pi^2}{K} \sum_{\langle \vec{r}, \vec{r}' \rangle} [\vec{\phi}(\vec{r}) - \vec{\phi}(\vec{r}')]^2 \right. \\ \left. + 2y_0 \sum_{\vec{r}} \{ \cos[2\pi \vec{e}_a \cdot \vec{\phi}(\vec{r})] \right. \\ \left. + \cos[2\pi \vec{e}_b \cdot \vec{\phi}(\vec{r})] \right. \\ \left. + \cos[2\pi \vec{e}_c \cdot \vec{\phi}(\vec{r})] \} \right). \quad (3.16)$$

In Appendix B, we gauge the importance of the periodic part of (3.14) by examining its auto-correlation in the limit  $y_0 = 0$ . These correlations decay as power laws at large distances, and indicate that the renormalization-group eigenvalue of  $y_0$  is

$$\lambda_{y_0} = 2 - \bar{K}/8\pi. \quad (3.17)$$

An identical result holds for all Bravais lattices with  $|\vec{e}_1| = |\vec{e}_2|$  and  $-1 < \vec{e}_1 \cdot \vec{e}_2 < 1$ . According to renormalization theory,<sup>40</sup> dislocations grow in importance with repeated iterations of a renormalization-group transformation whenever  $\lambda_{y_0} > 0$ , but fade into insignificance for  $\lambda_{y_0} < 0$ . Consequently, we expect that dislocations will be unimportant at low temperatures, but that they will ultimately cause a transition into some new kind of behavior for

$$\bar{K} \lesssim 16\pi. \quad (3.18)$$

Dislocations with larger Burger's vectors may

also be represented as periodic perturbations to the Gaussian part of (3.12), but with a period that is shorter than that of the terms exhibited in (3.14). A calculation of the eigenvalue analogous to (3.17) shows that these excitations become relevant only at temperatures much higher than the temperature at which the lowest-lying dislocations become important.

### C. Duality and bond moving

If the angular part of  $\vec{\phi}_D$  can indeed be ignored, and if the Burger's excitations form a square lattice, the dislocation partition sum  $Z_c$  factors into the partition functions of two independent Coulomb gases. The local formulation (3.6) of melting also decouples in this limit, although a nontrivial coupling is apparently introduced whenever  $\vec{e}_1 \cdot \vec{e}_2 \neq 0$ . Since a scalar Coulomb gas is supposed to be in the same universality class as the two-dimensional planar model,<sup>15, 23, 24</sup> one might expect that  $Z'_c$  is in some sense equivalent to two coupled planar models.

An approximate equivalence of melting to two coupled planar models or "superfluids" is also suggested by the definition (2.5) of the Burger's vector of a dislocation. The form of  $\vec{b}(\vec{r})$  makes it tempting to write

$$\vec{u}(\vec{r}) = [a_0 \theta_1(\vec{r})/2\pi] \vec{e}_1 + [a_0 \theta_2(\vec{r})/2\pi] \vec{e}_2, \quad (3.19)$$

where  $\theta_1(\vec{r})$  and  $\theta_2(\vec{r})$  are the phases associated with complex wave functions  $\psi_1(\vec{r})$  and  $\psi_2(\vec{r})$ . Indeed, deGennes and McMillan have proceeded in a similar fashion to draw a detailed analogy between smectic-A liquid crystals and superconductors.<sup>41, 42</sup> Although the coupling between space and the displacement field present in (2.4) complicates the analysis in the present case, it is not hard to find models of this kind which are in fact closely related to (3.6).

Consider, for example, two such "superfluids" or XY models embedded in a square lattice of

sites  $\vec{R}$ , with a reduced Hamiltonian

$$\mathcal{H}_s \equiv \sum_{\langle \vec{R}, \vec{R}' \rangle} V(\theta_1(\vec{R}) - \theta_1(\vec{R}'), \theta_2(\vec{R}) - \theta_2(\vec{R}')), \quad (3.20)$$

where  $V(\theta_1, \theta_2)$  is periodic function of its arguments:

$$V(\theta_1 + 2\pi m, \theta_2 + 2\pi n) = V(\theta_1, \theta_2), \quad (3.21)$$

$$m = 0, \pm 1, \dots, \quad n = 0, \pm 1, \dots,$$

and the summation is restricted to nearest-neighbor lattice sites. A potential function  $V(\theta_1, \theta_2)$  which turns out to correspond rather closely to melting is

$$V(\theta_1(\vec{R}) - \theta_1(\vec{R}'), \theta_2(\vec{R}) - \theta_2(\vec{R}')) = (J/k_B T) \{ \text{Re}[\psi_1(\vec{R})\psi_1^*(\vec{R}') + \psi_2(\vec{R})\psi_2^*(\vec{R}')] + 2g \text{Im}[\psi_1(\vec{R})\psi_1^*(\vec{R}')] \times \text{Im}[\psi_2(\vec{R})\psi_2^*(\vec{R}')] \}, \quad (3.22a)$$

where

$$\psi_1(\vec{R}) \equiv e^{i\theta_1(\vec{R})}, \quad \psi_2(\vec{R}) = e^{i\theta_2(\vec{R})} \quad (3.22b)$$

There is a "current-current" coupling between  $\psi_1$  and  $\psi_2$ . We allow no explicit dependence on the magnitudes of  $\psi_1(\vec{R})$  and  $\psi_2(\vec{R})$  in  $\mathcal{H}_s$ , which is consistent with recent studies of magnetism and superfluidity in  $2 + \epsilon$  dimensions.<sup>17-20</sup> This work suggests that fluctuations in the magnitude of the order parameter are unimportant at all temperatures below  $T_c$  for  $n=2$  component spins and superfluids.<sup>43</sup>

To see that (3.17) is related to (3.6), one can proceed exactly as in Sec. II B of Ref. 24 to carry out a series of duality transformations or  $\overline{\mathcal{H}}_s$ .<sup>44</sup> The result is that the partition sum,

$$Z_s \equiv \left( \prod_{\vec{R}} \int_0^{2\pi} \frac{d\theta_1(\vec{R})}{2\pi} \int_0^{2\pi} \frac{d\theta_2(\vec{R})}{2\pi} \right) e^{\overline{\mathcal{H}}_s} \quad (3.23)$$

can be reexpressed in terms of the Fourier transform  $e^{\tilde{V}(p,q)}$  of  $e^{V(\theta_1, \theta_2)}$  by

$$Z_s = \sum_{\{p(\vec{r})=-\infty\}} \sum_{\{q(\vec{r})=-\infty\}} \exp \left[ \sum_{\langle \vec{r}, \vec{r}' \rangle} \tilde{V}(p(\vec{r}) - p(\vec{r}'), q(\vec{r}) - q(\vec{r}')) \right], \quad (3.24)$$

where

$$e^{\tilde{V}(p,q)} = \int_0^{2\pi} \frac{d\theta_1}{2\pi} \int_0^{2\pi} \frac{d\theta_2}{2\pi} \exp V[\theta_1, \theta_2] \times \exp[-i\theta_1 p - i\theta_2 q], \quad (3.25)$$

and  $p(\vec{r})$  and  $q(\vec{r})$  are integer-valued variables occupying the sites  $\vec{r}$  of the lattice dual to the sites  $\vec{R}$ . Evidently,  $Z_s$  will be identical to a vector Coulomb-gas partition function  $Z'_c$  provided  $\tilde{V}(p, q)$  takes the form

$$\tilde{V}(p, q) = -[4\pi^2/\bar{K}(1-x^2)](p^2 + q^2 - 2xpq) \quad (3.26)$$

for some  $\bar{K}$  and  $x$ . A rough calculation shows that the Fourier transform of (3.22a) assumes this form at low temperatures, with  $J/k_B T \approx \bar{K}(1-x^2)/8\pi^2$  and  $q \approx x$ .

The connection between two coupled superfluids and melting, as well as the global universality of the description (3.6), can be explored further using an approximate renormalization-group recursion scheme due to Migdal.<sup>18</sup> According to Kadanoff's reformulation<sup>26</sup> of this approach, one can construct approximate recursion relations by first moving nearest-neighbor interactions as shown in Fig. 2(a), and then integrating over a "one dimensional" subset of the degrees of freedom. The transformation is completed by rotating the lattice

by 90° and repeating the procedure. Alternatively, one can obtain essentially the same recursion formulas by first moving both  $x$  and  $y$  bonds at once, as suggested by Fig. 2(b).<sup>45</sup> Recursion

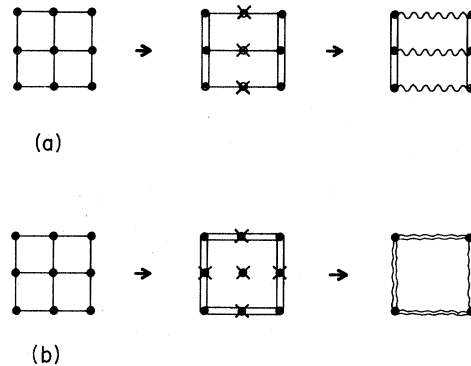


FIG. 2. Schematic representation of Migdal's approximate renormalization-group procedure, as reformulated by Kadanoff. In Fig. 2(a), vertical bonds are first moved sideways to create isolated "one-dimensional" degrees of freedom marked by a  $\times$ . After integrating over these variables, one obtains a rectangular lattice with half as many degrees of freedom. The transformation is completed by turning the lattice on its side and repeating the procedure. Figure 2(b) shows a one-step version of this transformation which leads to essentially the same recursion relation. Both horizontal and vertical bonds are first moved, followed by a "decimation" of the degrees of freedom marked by an  $\times$ .



relations are easily constructed in this fashion from (3.19), or by performing partial traces over the dual degree's of freedom displayed in (3.21). Crude as it is, this procedure is known to give remarkably good results in situations where fluctuations have destroyed conventional long-range order. When applied to the two-dimensional planar model,<sup>18,24</sup> this approach gives results almost indistinguishable from the line of critical points with continuously variable exponents (corresponding to a line of fixed points) present in Kosterlitz' more exact analysis.<sup>23</sup>

Working in the space of angular variables, using the scheme summarized in Fig. 2(b), we find that recursion relations for the Fourier components of the potential may be written

$$e^{\tilde{V}'(p,q)} = \left( \sum_{p_1=-\infty}^{\infty} \sum_{q_1=-\infty}^{\infty} \exp \tilde{V}(p_1, q_1) \times \exp \tilde{V}(p - p_1, q - q_1) \right)^2. \quad (3.27a)$$

Carrying out the Migdal-Kadanoff procedure in the dual space of integer-valued variables, one obtains

$$e^{\tilde{V}'(p,q)} = \sum_{p_1=-\infty}^{\infty} \sum_{q_1=-\infty}^{\infty} \exp 2\tilde{V}(p_1, q_1) \times \exp 2\tilde{V}(p - p_1, q - q_1). \quad (3.27b)$$

Although (3.27a) and (3.27b) lead to qualitatively similar results, we have worked primarily with Eq. (3.27b).

A numerical analysis of (3.27b) with a variety of initial coupling functions  $V(\theta_1, \theta_2)$  reveals that such couplings rapidly collapse (in practice, after four or five iterations of the transformation) to a two-parameter family of functions with Fourier components of the form (3.26). This rapid collapse strongly suggests that the partition function  $Z_s$  for two coupled superfluids will display singularities identical to those associated with the vector Coulomb-gas partition sum  $Z'_c$ .

We have explored in some detail the action of (3.27b) on initial couplings of the form (3.26). There is an apparent surface of fixed points bounded by a line  $\bar{K}_m^{-1}(x)$ , which we associate with a locus of melting transitions (see Fig. 3). The low-temperature shaded region of fixed points in this figure presumably corresponds to a solid phase. Fixed point functions  $V^*(\theta_1, \theta_2)$  in this region for a square ( $x=0$ ) and triangular ( $x=\frac{1}{2}$ ) lattice of excitations are shown in Fig. 4. Hamiltonians in the high-temperature or "fluid" region of Fig. 3 iterate rapidly toward an infinite-temperature fixed point where all Fourier components except  $V(0,0)$  are zero. As was the case for the

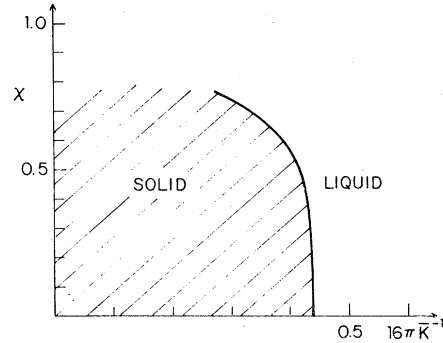


FIG. 3. Phase diagram for melting obtained from the Migdal procedure as a function of the temperaturelike variable  $16\bar{K}^{-1}$  and  $x = \vec{e}_1 \cdot \vec{e}_2$ , the dot product of the basis vectors of the Bravais crystalline lattice. The Hamiltonians in the shaded region are attracted to an apparent surface of fixed points. Although the analysis of Sec. IV suggests that melting is indeed described by such a fixed surface, the approximate Migdal recursion relations display an exponentially small ( $\sim e^{-c\bar{K}}$ ) drift toward higher temperatures even in the shaded region. We regard this drift as an artifact of the approximation, and estimate a locus of melting temperatures  $\bar{K}_m^{-1}(x)$  separating the fluid and solid phases by the condition that the fractional change of  $e^{\tilde{V}(0,0)}$  in one iteration equals 0.005. The melting temperatures  $\bar{K}_m^{-1}(x)$  obtained in this way remains approximately constant as  $x$  varies from zero (square lattice) to  $\frac{1}{2}$  (triangular lattice), and then begins to decrease. The behavior for  $x \geq 0.7$  was not investigated in detail.

two-dimensional planar model,<sup>24</sup> a more careful analysis of the Migdal-Kadanoff transformation shows that the fixed points in Fig. 3 are only apparent—at any finite  $\bar{K}^{-1} > 0$ , there is an exponentially small (in  $1/T$ ) drift of Hamiltonians toward

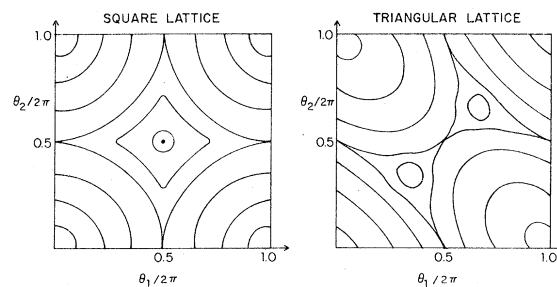


FIG. 4. Fixed-point potentials  $V^*(\theta_1, \theta_2)$  which arise from a representation of melting in terms of two coupled superfluids for (a) square and (b) triangular lattices. There are minima at the four corners of the squares in both figures, and saddle points along the four sides. Figure 4(a) has a maximum at the center, while Fig. 4(b) has two maxima separated by a saddle point. All fixed-point potentials along the lines  $x=0$  and  $x=\frac{1}{2}$  in Fig. 3 have the shapes shown in Figs 4(a) and 4(b), respectively.

high temperatures with repeated iterations of the transformation. We regard this (virtually undetectable) drift as an artifact of the approximation procedure, and shall argue in Sec. IV that melting in two dimensions is in fact characterized by a two-dimensional "surface" of fixed points.

The "fixed surface" which is swept out as  $x$  varies from zero to unity in Fig. 3 is reminiscent of the fixed line (with continuously variable critical exponents) generated by varying the four-spin coupling in the Kadanoff-Wegner reformulation<sup>46</sup> of the Baxter model.<sup>47</sup> The potential (3.18a) is written in a way which reinforces this analogy. Taking over a trick used in Ref. 46 we can show analytically that  $x$  is a marginal operator at every point along the line of fixed points present for  $x=0$ :

Consider the reduced Hamiltonian associated with (3.6),

$$\bar{\mathcal{H}}'_c = \bar{\mathcal{H}}_p + \bar{\mathcal{H}}_q + \left[ \frac{8\pi^2 x}{\bar{K}(1-x^2)} \right] \sum_{\vec{r}} O(\vec{r}), \quad (3.28)$$

where

$$\bar{\mathcal{H}}_p = -[4\pi^2/\bar{K}(1-x^2)] \sum_{\langle \vec{r}, \vec{r}' \rangle} [p(\vec{r}) - p(\vec{r}')]^2, \quad (3.29a)$$

$$\bar{\mathcal{H}}_q = -\left[ \frac{4\pi^2}{\bar{K}(1-x^2)} \right] \sum_{\langle \vec{r}, \vec{r}' \rangle} [q(\vec{r}) - q(\vec{r}')]^2, \quad (3.29b)$$

and we want to assess the importance of the density

$$O(\vec{r}) = \sum_{\vec{\delta}} [p(\vec{r}) - p(\vec{r} + \vec{\delta})][q(\vec{r}) - q(\vec{r} + \vec{\delta})]. \quad (3.30)$$

The summation in (3.27) runs over unit vectors  $\vec{\delta}_1 = (1, 0)$  and  $\vec{\delta}_2 = (0, 1)$  connecting nearest-neighbor lattice sites. According to a criterion proposed by Kadanoff,<sup>40</sup> the importance of  $O(\vec{r})$  can be gauged by examining a correlation function evaluated at  $x=0$  (see Appendix B), namely,

$$C(\mathbf{r}_1 - \mathbf{r}_2) \equiv \langle O(\mathbf{r}_1) O(\mathbf{r}_2) \rangle_{\bar{\mathcal{H}}_p + \bar{\mathcal{H}}_q}. \quad (3.31)$$

Substituting (3.30) into (3.31), we can estimate  $C(\vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2)$  at large  $|\vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2|$ ,

$$\begin{aligned} C(\mathbf{r}_1 - \mathbf{r}_2) &= \left[ \sum_{\vec{\delta}, \vec{\delta}'} \langle [p(\vec{\mathbf{r}}_1) - p(\vec{\mathbf{r}}_1 + \vec{\delta})] \right. \\ &\quad \left. \times [p(\vec{\mathbf{r}}_2) - p(\vec{\mathbf{r}}_2 + \vec{\delta}')] \rangle_{\bar{\mathcal{H}}_p} \right]^2, \\ &\approx \left[ \sum_{\vec{\delta}, \vec{\delta}'} \delta_i \delta_j \frac{\partial^2}{\partial r_{1i} \partial r_{2j}} \right. \\ &\quad \left. \times \langle p(\vec{\mathbf{r}}_1) p(\vec{\mathbf{r}}_2) \rangle_{\bar{\mathcal{H}}_p} \right]^2. \end{aligned} \quad (3.32)$$

Provided dislocations are sufficiently dilute, we

can determine  $\langle p(\vec{\mathbf{r}}_1) p(\vec{\mathbf{r}}_2) \rangle_{\bar{\mathcal{H}}_p}$  simply by integrating rather than summing over the variables  $p(\vec{\mathbf{r}})$ . At large  $|\vec{\mathbf{r}} - \vec{\mathbf{r}}'|$ , we find

$$\langle p(\vec{\mathbf{r}}_1) p(\vec{\mathbf{r}}_2) \rangle \sim \ln |\vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2|, \quad (3.33)$$

so that

$$C(\vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2) \sim 1/|\vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2|^4 \quad (3.34)$$

as  $|\mathbf{r}_1 - \mathbf{r}_2| \rightarrow \infty$  independent of the value of  $\bar{K}$ . Following the discussion in Appendix B, we conclude that  $O(\vec{r})$  is a marginal operator for *all* values of  $\bar{K}^{-1}$  less than  $\bar{K}_m^{-1}(0)$ , as suggested by the apparent surface of fixed points displayed in Fig. 3.

#### IV. SCALING EQUATIONS

In principle, corrections to results such as (3.1) and (3.2) for correlations between Burger's vectors can be determined by perturbation theory in  $y$ . Such a perturbation series breaks down, however, at sufficiently high temperatures. Difficulties in the perturbative calculation of correlations can be overcome with a renormalization procedure similar to that developed by Kosterlitz<sup>23</sup> and by José *et al.*<sup>24</sup>. As a byproduct of the calculations, we obtain as a perturbation series in  $\bar{y}$  recursion relations or "scaling equations" for melting which complement the nonperturbative, but approximate, renormalization-group equations studied in Sec. III. The calculations will be carried out neglecting the angular factors discussed in Sec. III A. As we shall see, the probability  $\bar{y}$  of a dislocation pair excitation is driven to zero below  $T_m$ , so that a purely harmonic theory of phonons with no dislocations should become arbitrarily accurate at long wavelengths.

##### A. Scaling equations for the square lattice

Consider the correlation functions

$$\Gamma_b(\mathbf{r}_{12}, \bar{K}, \bar{y}) \equiv \langle \vec{\mathbf{b}}(\vec{\mathbf{r}}_1) \cdot \vec{\mathbf{b}}(\vec{\mathbf{r}}_2) \rangle_C, \quad (4.1)$$

where  $\mathbf{r}_{12} = |\vec{\mathbf{r}}_1 - \vec{\mathbf{r}}_2|$ , and the average is evaluated in the vector Coulomb-gas ensemble (3.3). If the allowed Burger's vectors form a square lattice,  $\bar{\mathcal{H}}_c$  breaks into two decoupled scalar Coulomb gases, and we can write

$$\begin{aligned} \Gamma_b(\mathbf{r}_{12}, \bar{K}, \bar{y}) &= 2\Gamma_m(\mathbf{r}_{12}, \bar{K}, \bar{y}) \\ &\equiv 2\langle m(\mathbf{r}_1) m(\mathbf{r}_2) \rangle_{sc}, \end{aligned} \quad (4.2)$$

where  $m(\vec{\mathbf{r}}) = 0, \pm 1, \pm 2, \dots$ , and the average is evaluated in a scalar Coulomb (sC) gas ensemble with probability proportional to  $e^{\bar{\mathcal{H}}_{sc}}$ ,

$$\mathcal{Z}_{\text{sc}} = \frac{K}{8\pi} \int \frac{d^2r}{a^2} \int_{|\vec{r}-\vec{r}'|>a} \frac{d^2r'}{a^2} m(\vec{r})m(\vec{r}') \times \ln(|\vec{r}-\vec{r}'|/a) + \ln(y) \int \frac{d^2r}{a^2} m^2(\vec{r}). \quad (4.3)$$

In evaluating averages, we sum only over those complexions of integers which satisfy the charge-conservation condition  $\int d^2r m(\vec{r})=0$ . Although the scaling equations for a scalar Coulomb gas are quite well known from studies of the XY model

$$\Gamma_2(r_{12}, \bar{K}) = -2(r_{12}/a)^{-\alpha}, \quad (4.5a)$$

$$\Gamma_4(r_{12}, \bar{K}) = -2\left(\frac{r_{12}}{a}\right)^{-\alpha} \int \frac{d^2r_a}{a^2} \int \frac{d^2r_b}{a^2} \left(\frac{|r_a - r_b|}{a}\right)^{-\alpha} \exp[-\alpha g(\vec{r}_1 - \vec{r}_a) + \alpha g(r_1 - r_b) + \alpha g(r_2 - r_a) - \alpha g(r_2 - r_b)], \quad (4.5b)$$

and where we have introduced the abbreviations

$$\alpha = K/4\pi, \quad g(\vec{r}) = \ln(|\vec{r}|/a). \quad (4.6)$$

The quantities  $\Gamma_2(r_{12}, \bar{K})$  and  $\Gamma_4(r_{12}, \bar{K})$  come from the configurations of  $m(\vec{r})$  excitations shown in Figs. 5(a) and 5(b). Two excitations with  $m(\vec{r}) = \pm 1$  are anchored at  $\vec{r}_1$  and  $\vec{r}_2$ , while we integrate freely over the excitations at  $\vec{r}_a$  and  $\vec{r}_b$  in Fig. 5(b). As suggested by this figure, we expect that the renormalization of  $\Gamma_m(r, \bar{K}, \bar{y})$  will be dominated by tightly-bound pairs of excitations. Another tightly bound configuration associated with (4.5b), together with a complexion that cancels it to lowest order, is shown in Fig. 5(c). The scalar Coulomb-gas partition sum which enters (4.4) will be needed to  $O(\bar{y}^4)$ ,

$$Z_{\text{sc}} = 1 + 2 \frac{\Omega}{a^2} \bar{y}^2 \int_{|\vec{r}|>a} \frac{d^2r}{a^2} \left(\frac{r}{a}\right)^{-\alpha} + O(\bar{y}^4), \quad (4.7)$$

where  $\Omega$  is the area of the system.

The expression for  $\Gamma(r, \bar{K})$  can be simplified by assuming that the renormalization of  $\Gamma_m(r, \bar{K}, \bar{y})$  is dominated by configurations with  $\vec{r}_a$  very close to  $\vec{r}_b$ . On changing integration variables to

$$\begin{aligned} \vec{R} &= \frac{1}{2}(\vec{r}_a + \vec{r}_b), \\ \vec{r} &= \vec{r}_a - \vec{r}_b, \end{aligned} \quad (4.8)$$

and expanding in  $\vec{r}$ , the exponentiated part of  $\Gamma_4$  can be rewritten,

$$\begin{aligned} &\exp[-\alpha g(\vec{r}_1 - \vec{r}_a) + \alpha g(\vec{r}_1 - \vec{r}_b) + \alpha g(\vec{r}_2 - \vec{r}_a) \\ &\quad - \alpha g(\vec{r}_2 - \vec{r}_b)] \\ &\approx \exp\{\alpha \vec{r} \cdot \nabla_{\vec{R}} [g(\vec{r}_1 - \vec{R}) - g(\vec{r}_2 - \vec{R})]\}. \end{aligned} \quad (4.9)$$

model,<sup>23,25</sup> it is interesting to see how they arise from a consideration of the correlation function (4.2). The same calculational procedure is applied to the more-interesting problem of a triangular lattice of Burger's vectors in Sec. IV B. The perturbation expansion in  $\bar{y}$  for  $\Gamma_m(r_{12}, \bar{K}, \bar{y})$  takes the form

$$\Gamma_m(r_{12}, \bar{K}, \bar{y}) = Z_{\text{sc}}^{-1} [\Gamma_2(r_{12}, \bar{K}) \bar{y}^2 + \Gamma_4(r_{12}, \bar{K}) \bar{y}^4 + O(\bar{y}^6)], \quad (4.4)$$

where

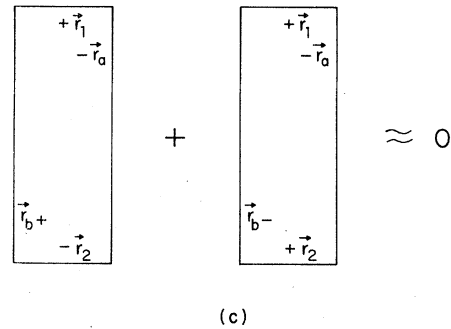
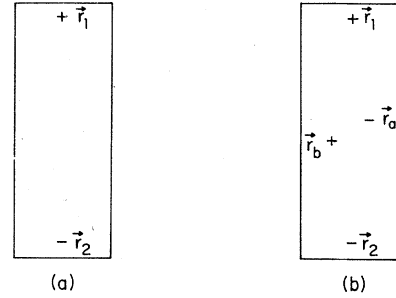


FIG. 5. Configurations of excitations which enter the correlation function  $\Gamma_m(r_{12}, \bar{K}, \bar{y})$  for the scalar Coulomb gas. The complexions which contribute to  $\Gamma_2(r_{12}, \bar{K})$  and  $\Gamma_4(r_{12}, \bar{K})$  are shown in Figs. 5(a) and 5(b), respectively. As suggested by Fig. 5(b), the important part of  $\Gamma_4(r_{12}, \bar{K})$  comes when  $\vec{r}_a$  is close to  $\vec{r}_b$ . The "disconnected" part of  $\Gamma_4(r_{12}, \bar{K})$  which occurs when  $\vec{r}_a$  is very close  $\vec{r}_1$  and  $\vec{r}_b$  is very close to  $\vec{r}_2$  is canceled by another complexion of four excitations, as shown in Fig. 5(c).

Expanding the exponential to second order in  $\vec{r}$ , and carrying out the angular average over  $\vec{R}$ , we find

$$\Gamma_4(r_{12}, \bar{K}) = -2 \left( \frac{r_{12}}{a} \right)^{-\alpha} \int \frac{d^2 r}{a^2} \int \frac{dR}{a^2} \left( \frac{r}{a} \right)^{-\alpha} \left\{ 1 + \frac{1}{4} \alpha^2 r^2 \left| \vec{\nabla}_R [g(\vec{r}_1 - \vec{R}) - g(\vec{r}_2 - R)] \right|^2 \right\} \quad (4.10)$$

which simplifies after a partial integration to

$$\begin{aligned} \Gamma_4(r_{12}, K) = & -2(r_{12}/a)^{-\alpha} \\ & \times \left[ \frac{\Omega}{a^2} \int_{|\vec{r}|>a} \frac{d^2 r}{a^2} \left( \frac{r}{a} \right)^{-\alpha} \right. \\ & \left. + 2\pi^2 \alpha^2 g(r_{12}) \int_a^\infty \frac{dr}{a} \left( \frac{r}{a} \right)^{3-\alpha} \right]. \end{aligned} \quad (4.11)$$

We have cut off the integrations over  $\vec{r}$  at the core size  $a$ , and made use of the identity  $\nabla^2 g(\vec{r}) = 2\pi\delta(\vec{r})$ .

Collecting together the various contributions to  $\Gamma_m(r_{12}, \bar{K}, \bar{y})$ , we find that the terms proportional to the area of the system in (4.7) and (4.11) cancel, and that

$$\begin{aligned} \Gamma_m(r_{12}, \bar{K}, \bar{y}) = & -2y^2 e^{-\alpha g(r_{12})} \\ & \times \left[ 1 + 2\pi^2 \alpha^2 \bar{y}^2 \ln[g(\vec{r}_{12})] \right. \\ & \left. \times \int_a^\infty \frac{dr}{a} \left( \frac{r}{a} \right)^{3-\alpha} + O(\bar{y}^4) \right]. \end{aligned} \quad (4.12)$$

To  $O(\bar{y}^4)$ , we can exponentiate the logarithm in (4.12) and find that  $\Gamma_m(r_{12}, \bar{K}, \bar{y})$  takes the form

$$\Gamma_m(r_{12}, \bar{K}, \bar{y}) = -2y^2 (r_{12}/a)^{-K} e^{rt/4\pi}, \quad (4.13)$$

where

$$\bar{K}_{\text{eff}} = \bar{K} - \frac{1}{2} \pi \bar{K}^2 \bar{y}^2 \int_a^\infty \frac{dr}{a} \left( \frac{r}{a} \right)^{3-\bar{K}/4\pi}, \quad (4.14)$$

and we have made use of the definition (4.6) of  $\alpha$ . Although (4.14) correctly gives the modification in  $\Gamma_m(r, \bar{K}, \bar{y})$  due to screening by dislocation pairs at low temperatures, difficulties arise when  $\bar{K}$  approaches  $16\pi$ , since the integral then becomes very large. Following José *et al.*,<sup>24</sup> we study this problem by splitting the integrals over  $r$  into two parts

$$\int_a^\infty \frac{dr}{a} \rightarrow \int_a^{ae^l} \frac{dr}{a} + \int_{ae^l}^\infty \frac{dr}{a}, \quad (4.15)$$

and absorbing the small- $r$  integrations into a redefinition of  $\bar{K}$ . Upon rescaling the remaining integrations so that the large  $r$  integrals again run from  $a$  to  $\infty$ , we find that (4.14) can be rewritten in the form

$$\begin{aligned} \bar{K}_{\text{eff}} = & \bar{K}' - \frac{1}{2} \pi (\bar{K}')^2 (\bar{y}')^2 \\ & \times \int_a^\infty \frac{dr}{a} \left( \frac{r}{a} \right)^{3-\bar{K}'/4\pi} + O((\bar{y}')^4), \end{aligned} \quad (4.16)$$

with

$$\bar{K}' = \bar{K} - \frac{1}{2} \pi \bar{K}^2 \bar{y}^2 \int_a^{ae^l} \frac{dr}{a} \left( \frac{r}{a} \right)^{3-\bar{K}/4\pi}, \quad (4.17a)$$

$$\bar{y}' = e^{(2-\bar{K}/8\pi)l} \bar{y}. \quad (4.17b)$$

Setting  $l = \delta$  and letting  $\delta \rightarrow 0$ , we can easily construct differential recursion or scaling equations from (4.16) and (4.17). After length scales between  $a$  and  $ae^l$  have been integrated out, the series (4.16) takes the form

$$\bar{K}_{\text{eff}} = \bar{K}(l) - \frac{1}{2} \pi \bar{K}^2(l) \bar{y}^2(l) \int_a^\infty \frac{dr}{a} \left( \frac{r}{a} \right)^{3-\bar{K}(l)/4\pi}, \quad (4.18)$$

with

$$\frac{d\bar{K}^{-1}(l)}{dl} = \frac{1}{2} \pi \bar{y}^2(l) + O(\bar{y}^4(l)), \quad (4.19a)$$

$$\frac{d\bar{y}(l)}{dl} = [2 - \bar{K}(l)/8\pi] \bar{y}(l) + O(\bar{y}^3(l)), \quad (4.19b)$$

and  $\bar{K}(l=0) = \bar{K}$ ,  $\bar{y}(l=0) = \bar{y}$ . Applying the same procedure to the series (4.12), we obtain the behavior of  $\Gamma_m(r_{12}, \bar{K}, \bar{y})$  under the renormalization-group procedure,

$$\Gamma_m(r_{12}, \bar{K}, \bar{y}) = e^{-4l} \Gamma_m(e^{-l} r_{12}, \bar{K}(l), \bar{y}(l)). \quad (4.20)$$

The familiar Hamiltonian flows associated with (4.19) are displayed in Fig. 6(a). The low-temperature crystalline phase is associated with the set of trajectories which approach the line of fixed points at  $\bar{y} = 0$ . A typical locus of initial Hamiltonians given by (3.4) with  $C = 3$  is shown as a dashed line. The intersection of this line with the incoming separatrix determines the melting temperature. The dislocation probability  $\bar{y}(l)$  appears to grow without bound to the right of this separatrix, presumably signaling the dissociation of dislocation pairs predicted by Kosterlitz and Thouless.<sup>15</sup>

## B. Scaling equations for the triangular lattice

Since  $\mathcal{H}_c$  does not break into two decoupled scalar Coulomb gases when the allowed excitations form a triangular lattice, the derivation of scaling equations is somewhat more complicated. The perturbation series for  $\Gamma_b(r_{12}, \bar{K}, \bar{y})$  now takes the form

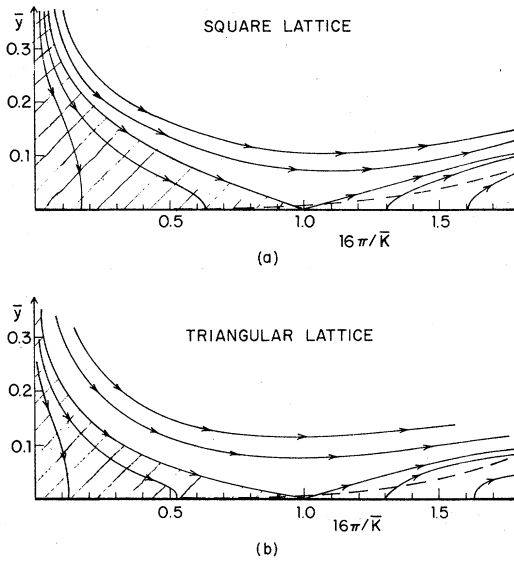


FIG. 6. Hamiltonian flows induced by the scaling equations for melting of (a) square and (b) triangular lattices. Typical loci of initial conditions are shown as dashed lines. Hamiltonians which start in the shaded region are mapped by the renormalization transformation into the line of fixed points at  $\bar{y}=0$ . Dislocations become unimportant at long wavelengths in this region, which we identify with a crystalline phase. Dislocations ultimately increase in importance in the remainder of the  $\bar{K}^{-1}-\bar{y}$  plane, which we identify with a fluid phase. The fixed lines at  $\bar{y}=0$  represent two cross sections of the fixed surface shown in Fig. 3.

$$\Gamma_b(r_{12}, \bar{K}, \bar{y}) = Z_c^{-1} [\Gamma_2(r_{12}, \bar{K}) \bar{y}^2 + \Gamma_3(r_{12}, \bar{K}) \bar{y}^3 + \Gamma_4(r_{12}, \bar{K}) \bar{y}^4 + O(\bar{y}^5)], \quad (4.21)$$

with

$$\Gamma_2(r_{12}, \bar{K}) = -6(r_{12}/a)^{-\alpha}, \quad (4.22a)$$

$$\Gamma_3(r_{12}, \bar{K}) = -6 \left( \frac{r_{12}}{a} \right)^{-1/2\alpha} \times \int \frac{d^2 r}{a^2} \exp[-\frac{1}{2} \alpha g(\bar{r} - \bar{r}_1) - \frac{1}{2} \alpha g(\bar{r} - \bar{r}_2)], \quad (4.22b)$$

and where  $\Gamma_4(r_{12}, \bar{K})$  can be written

$$\Gamma_4(r_{12}, \bar{K}) = -6 [\Gamma_{4,1}(r_{12}, \bar{K}) + 2\Gamma_{4,2}(r_{12}, \bar{K})]. \quad (4.22c)$$

The contribution to  $\Gamma_3(r_{12}, \bar{K})$  comes from three dislocations, with Burger's vectors oriented at

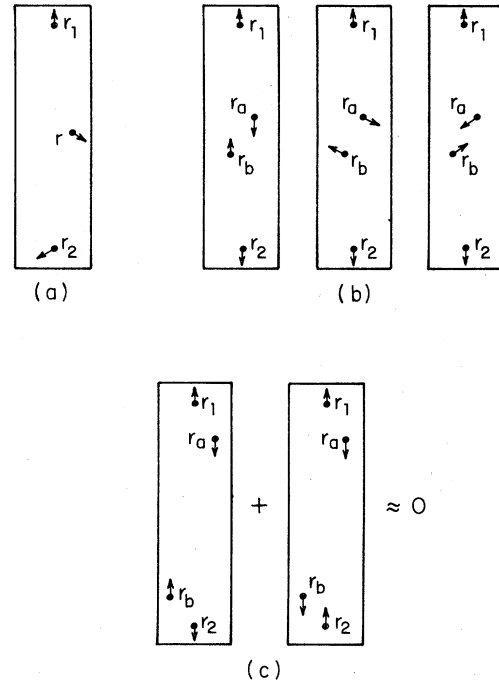


FIG. 7. Configurations of dislocations which contribute to  $\Gamma_b(r_{12}, \bar{K}, \bar{y})$  for melting on a triangular lattice. The order- $\bar{y}^2$  contribution is not shown while Fig. 7(a) shows one of the 12 complexions which occur at  $O(\bar{y}^3)$ . The dominant part of  $\Gamma_3(r_{12}, \bar{K})$  occurs when  $\bar{r}$  is near  $\bar{r}_1$  or  $\bar{r}_2$ . Figure 7(b) shows the three dominant configurant configurations of four dislocations which enter at  $O(\bar{y}^4)$ . The first complexion gives a contribution  $\Gamma_{4,1}(r_{12}, \bar{K})$  while the second and third each give  $\Gamma_{4,2}(r_{12}, \bar{K})$ . The important parts of the integrations over  $\bar{r}_a$  and  $\bar{r}_b$  are again for  $\bar{r}_a$  close to  $\bar{r}_b$ . Contributions to the integrations where  $\bar{r}_a$  is close to  $\bar{r}_1$  and  $\bar{r}_b$  is close to  $\bar{r}_2$  is canceled by other configurations by Burger's vectors, as illustrated in Fig. 7(c).

$120^\circ$  to each other as shown in Fig. 7(a). Two of the dislocations are fixed at  $\bar{r}_1$  and  $\bar{r}_2$ , while the third is at a position  $\bar{r}$  over which we integrate freely. The configurations of four dislocations which dominate  $\Gamma_4(r_{12}, \bar{K})$  are shown in Fig. 7(b). Two dislocations are again anchored at  $\bar{r}_1$  and  $\bar{r}_2$ , although we integrate freely over the positions  $\bar{r}_a$  and  $\bar{r}_b$  of the remaining two. We again expect that the renormalization of  $\Gamma_b(r_{12}, \bar{K}, \bar{y})$  will be dominated by tightly-bound pairs of singularities. Other tightly bound complexions whose contributions cancel to lowest order are shown in Fig. 7(c). The first complexion shown in Fig. 7(b) contributes

$$\Gamma_{4,1}(\bar{r}_{12}) = \left( \frac{r_{12}}{a} \right)^{-\alpha} \int \frac{d^2 r_a}{a^2} \int \frac{d^2 r_b}{a^2} \left( \frac{|\bar{r}_a - \bar{r}_b|}{a} \right)^{-\alpha} \exp[-\alpha g(\bar{r}_1 - \bar{r}_a) + \alpha g(\bar{r}_1 - \bar{r}_b) + \alpha g(\bar{r}_2 - \bar{r}_a) - \alpha g(\bar{r}_2 - \bar{r}_b)], \quad (4.23)$$

while the second and third complexions each give a contribution

$$\Gamma_{4,2}(\vec{r}_{12}) = \left(\frac{r_{12}}{a}\right)^{-\alpha} \int \frac{d^2r_a}{a^2} \frac{d^2r_b}{a^2} \left(\frac{|\vec{r}_a - \vec{r}_b|}{a}\right)^{-\alpha} \exp\left[-\frac{1}{2}\alpha g(\vec{r}_1 - \vec{r}_a) + \frac{1}{2}\alpha g(\vec{r}_1 - \vec{r}_b) + \frac{1}{2}\alpha g(\vec{r}_2 - \vec{r}_a) - \frac{1}{2}\alpha g(\vec{r}_2 - \vec{r}_b)\right]. \quad (4.24)$$

The vector Coulomb-gas partition function is

$$Z_c = 1 + 6 \frac{\Omega}{a_2} \bar{y}^2 \int \frac{d^2r}{a^2} \left(\frac{r}{a}\right)^{-\alpha} + O(\bar{y}^4). \quad (4.25)$$

The quantity  $\Gamma_3(r_{12}, \bar{K})$  simplifies provided we suppose that  $r_{12} \gg a$  and assume that the integral is dominated by configurations with  $\vec{r}$  very close to  $\vec{r}_1$  or  $\vec{r}_2$ . If  $\vec{r}$  is near  $\vec{r}_1$ , for example, we have  $g(\vec{r} - \vec{r}_2) \approx g(\vec{r}_{12})$ . In this approximation,  $\Gamma_3(r_{12}, \bar{K})$  becomes

$$\Gamma_3(r_{12}, \bar{K}) = -24\pi \left(\frac{r_{12}}{a}\right)^{-\alpha} \int_a^\infty \frac{dr}{a} \left(\frac{r}{a}\right)^{1-\alpha/2}. \quad (4.26)$$

The contributions  $\Gamma_{4,1}(r_{12}, \bar{K})$  and  $\Gamma_{4,2}(r_{12}, \bar{K})$  can be simplified as in Sec. IV A to give

$$\begin{aligned} \Gamma_{4,1}(r_{12}, \bar{K}) &= \left(\frac{r_{12}}{a}\right)^{-\alpha} \left[ \frac{\Omega}{a^2} \int_{|\vec{r}| > a} \frac{d^2r}{a} \left(\frac{r}{a}\right)^{-\alpha} \right. \\ &\quad \left. + 2\pi^2 \alpha^2 g(\vec{r}_{12}) \right. \\ &\quad \left. \times \int_a^\infty \frac{dr}{a} \left(\frac{r}{a}\right)^{3-\alpha} \right], \end{aligned} \quad (4.27a)$$

$$\begin{aligned} \Gamma_{4,2}(r_{12}, \bar{K}) &= \left(\frac{r_{12}}{a}\right)^{-\alpha} \left[ \frac{\Omega}{a^2} \int_{|\vec{r}| > a} \frac{d^2r}{a} \left(\frac{r}{a}\right)^{-\alpha} \right. \\ &\quad \left. + \frac{1}{2} \pi^2 \alpha^2 g(\vec{r}_{12}) \right. \\ &\quad \left. \times \int_a^\infty \frac{dr}{a} \left(\frac{r}{a}\right)^{3-\alpha} \right]. \end{aligned} \quad (4.27b)$$

Collecting together the various contributions to  $\Gamma_b(r_{12}, K, y)$ , we find that the terms proportional to the area of the system again cancel, and that

$$\begin{aligned} \Gamma_b(r_{12}, \bar{K}, \bar{y}) &= -6\bar{y}^2 e^{-\alpha s(\vec{r}_{12})} \\ &\quad \times \left[ 1 + 4\pi\bar{y} \int_a^\infty \frac{dr}{a} \left(\frac{r}{a}\right)^{1-\alpha/2} \right. \\ &\quad \left. + 3\pi^2 \alpha^2 \bar{y}^2 \ln g(\vec{r}_{12}) \right. \\ &\quad \left. \times \int_a^\infty \frac{dr}{a} \left(\frac{r}{a}\right)^{3-\alpha} + O(\bar{y}^3) \right] \end{aligned} \quad (4.28)$$

As was the case for the scalar Coulomb gas, the integrals in (4.35) are poorly convergent for  $\alpha \geq 4$ . Again breaking the integrations in two parts, we discover that the small- $r$  portions of the  $O(\bar{y}^3)$  and  $O(\bar{y}^4)$  terms in (4.28) can be absorbed into additive renormalizations of  $\bar{y}$  and  $\bar{K}$ , respectively. On rescaling the integrations, we obtain (just as in Sec. IV A) differential recursion relations for  $\bar{K}(l) = 4\pi\alpha(l)$  and  $\bar{y}(l)$ , namely,

$$\frac{d\bar{K}^{-1}(l)}{dl} = \frac{3}{4} \pi \bar{y}^2(l) + O(\bar{y}^3(l)), \quad (4.29a)$$

$$\frac{d\bar{y}(l)}{dl} = \left( 2 - \frac{\bar{K}(l)}{8\pi} \right) \bar{y}(l) + 2\pi \bar{y}^2(l) + O(\bar{y}^3(l)). \quad (4.29b)$$

The transformation law for  $\Gamma_b(r_{12}, \bar{K}, \bar{y})$  under this procedure is

$$\begin{aligned} \Gamma_b(r_{12}, \bar{K}, \bar{y}) &= \exp\left(-4l - 4\pi \int_0^l \bar{y}(l') dl'\right) \\ &\quad \times \Gamma_b(e^{-l} r_{12}, \bar{K}(l), \bar{y}(l)). \end{aligned} \quad (4.30)$$

The initial conditions associated with (4.29) are, as usual,  $\bar{K}(l=0) = \bar{K}$ ,  $\bar{y}(l=0) = \bar{y}$ .

Hamiltonian flows generated by (4.30) are displayed in Fig. 6(b), together with a locus of initial Hamiltonians. Although there is now an asymmetry in the slopes of the incoming and outgoing separatrices, the qualitative picture of melting is the same as for a square lattice of excitations. For melting on more-general lattices, we find that the term  $2\pi\bar{y}^2(l)$  in (4.29b) is replaced by a term of order  $\bar{y}^{3-2(\epsilon_1 \cdot \epsilon_2)}$ . The surface of fixed points swept out as  $\vec{e}_1 \cdot \vec{e}_2$  is varied (Fig. 6 shows two cross sections of this surface) corresponding to the apparent fixed surface discovered using the Migdal transformation in Sec. III.

## V. SINGULARITIES NEAR MELTING

The scaling equations derived in Sec. IV predict a variety of singularities at the melting temperature. Because the equations appropriate for a square lattice have already been studied in detail by Kosterlitz, we will concentrate here on the predictions which follow from the more complicated triangular-lattice recursion relations.

### A. Correlation length

The structure factor of a two-dimensional crystal is proportional to

$$S(\vec{k}) \equiv \sum_{\vec{R}} e^{i\vec{k} \cdot \vec{R}} \langle \exp\{i\vec{k} \cdot [\vec{u}(\vec{R}) - \vec{u}(\vec{0})]\} \rangle, \quad (5.1)$$

where the sum is over the sites  $\vec{R}$  of a regular lattice, and the actual position  $\vec{r}$  of an atom in the crystal is  $\vec{r} = \vec{R} + \vec{u}(\vec{R})$ . In the harmonic approximation, which, as we have argued, becomes arbitrarily accurate in the low-temperature crystalline phase, the correlation function

$$C_{\vec{k}}(\vec{R}) \equiv \langle \exp\{i\vec{k} \cdot [\vec{u}(\vec{R}) - \vec{u}(\vec{0})]\} \rangle \quad (5.2)$$

decays as a power law with an exponent depending on temperature and the elastic constants.<sup>14</sup> This slow decay leads to a power-law singularity in  $S(\vec{k})$  as  $\vec{k}$  approaches a reciprocal-lattice point  $\vec{G}$ . For  $T > T_m$ , however, we expect an exponential decay of  $C_{\vec{k}}(\vec{R})$ ,

$$C_{\vec{k}}(\vec{R}) \sim e^{-|\vec{R}|/\xi_+}, \quad (5.3)$$

where the correlation length  $\xi_+$  diverges as  $T$  approaches  $T_m$  from above.

To determine the form of this divergence, we make use of the standard result<sup>40</sup> for the way in which  $\xi_+(K, y)$  transforms under a renormalization transformation, namely,

$$\xi_+(\bar{K}, \bar{y}) = e^l \xi_+(K(l), \bar{y}(l)). \quad (5.4)$$

As suggested by Fig. 8, the behavior of  $\xi_+$  as  $T \rightarrow T_m^+$  can be determined by integrating the scaling equations for  $\bar{K}(l)$  and  $\bar{y}(l)$  into the high-temperature fluid phase until  $l = l^*$  such that  $\bar{y}(l^*)$  equals, say,  $\frac{1}{10}$ . At this point,  $\xi_+(K(l^*), \frac{1}{10})$  is just some finite number, and we have from (5.4),

$$\xi(\bar{K}, \bar{y}) \sim e^{l^*}. \quad (5.5)$$

To determine  $l^*$ , it is necessary to study the

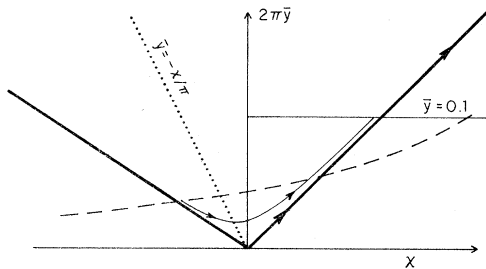


FIG. 8. Expanded version of the region about  $\bar{K} = 16\pi$  in Fig. 6(b). The correlation length and other functions of physical interest can be calculated by integrating along a renormalization-group trajectory from a point slightly above  $T_m$  on the dashed line until  $\bar{y}(l)$  equals, say, 0.1. At this point, one is sufficiently far from  $T_m$  to permit some approximate evaluation of the desired functions. As discussed in the text, different approximation schemes are used to integrate the scaling equations on the left and right sides of the dotted line  $\bar{y} = -x/\pi$ .

scaling equations in the vicinity of  $\bar{K} = 16\pi$ . To lowest order in a deviation  $x(l)$  defined by

$$\bar{K}^{-1}(l) = \frac{[1+x(l)]}{16\pi}, \quad (5.6)$$

the triangular-lattice recursion relations may be written

$$\frac{dx(l)}{dl} = 12\pi^2 \bar{y}^2(l), \quad (5.7a)$$

$$\frac{d\bar{y}(l)}{dl} = 2x(l)\bar{y}(l) + 2\pi\bar{y}^2(l). \quad (5.7b)$$

To find the incoming and outgoing separatrices in this approximation, we search for solutions of the form  $y(l) = mx(l)$ . There are two such straight-line trajectories, with slopes

$$m_+ = 1/2\pi, \quad m_- = -1/3\pi. \quad (5.8)$$

As shown in Fig. 8, a Hamiltonian which starts slightly above  $T_m$  will initially hug the incoming separatrix ( $m = m_-$ ), and then cross over and approach the outgoing separatrix ( $m = m_+$ ). According to (5.7b), the point where  $\bar{y}(l)$  stops decreasing and begins to increase is given by the intersection of a trajectory with the line

$$\bar{y} = -x/\pi. \quad (5.9)$$

The quantity  $l^*$  is conveniently calculated in two steps. We first determine the "time"  $l_1^*$  it takes for a trajectory to reach the line (5.9), and then estimate the "time"  $l_2^*$  it takes to go from this line to  $\bar{y}(l) = 0.1$ . Let us parametrize the trajectory of a Hamiltonian slightly above  $T_m$  by

$$\bar{y}(l) = -\frac{1}{3\pi} x(l) + D(l), \quad (5.10)$$

where the deviation  $D(l)$  from the incoming separatrix is initially small and proportional to  $(T - T_m)/T_m \equiv t$ ,

$$D(l=0) \equiv D_0 \propto t. \quad (5.11)$$

Inserting (5.10) into (5.7), we find that, for small deviations,

$$\frac{dD(l)}{dl} = -2x(l)D(l), \quad (5.12)$$

so that

$$D(l) = D_0 \exp\left(-2 \int_0^l x(l) dl\right). \quad (5.13)$$

To lowest order in  $D_0$ ,  $x(l)$  is given by the solution of

$$\frac{dx(l)}{dl} = \frac{4}{3} x^2(l), \quad (5.14)$$

namely,

$$x(l) = \frac{-|x_0|}{1 + \frac{4}{3}|x_0|l}, \quad (5.15)$$

where  $x_0$  is the negative initial value of  $x(l)$ . Combining (5.15) and (5.13), it follows that

$$D(l) = D_0(1 + \frac{4}{3}|x_0|l)^{3/2}. \quad (5.16)$$

The quantity  $l_1^*$  can now be determined by the requirement

$$\bar{y}(l_1^*) = -\frac{1}{3\pi} x(l_1^*) + D(l_1^*) = -\frac{1}{\pi} x(l_1^*). \quad (5.17)$$

Making use of (5.11), we find that the solution  $l_1^*$  of this equation may be written

$$l_1^* \approx C_1 t^{-2/5}, \quad (5.18)$$

where  $C_1$  is a nonuniversal constant.

To estimate  $l_2^*$ , we solve the equation for  $\bar{y}(l)$  along the outgoing separatrix,

$$\frac{d\bar{y}(l)}{dl} = 6\pi\bar{y}^2(l). \quad (5.19)$$

The solution with initial condition  $y_l = y(l_1^*)$  is

$$\bar{y}(l) = \frac{\bar{y}(l_1^*)}{1 - 6\pi\bar{y}(l_1^*)l}, \quad (5.20)$$

and it follows from (5.10) and (5.15) that  $\bar{y}(l_1^*) \approx 3/4\pi l_1^*$ . Imposing the requirement  $\bar{y}(l_2^*) = 0.1$  gives the result  $l_2^* \sim 1/\bar{y}(l_1^*) \sim l_1^*$ , so that

$$l_2^* \approx C_2 t^{-2/5}, \quad (5.21)$$

where  $C_2$  is another nonuniversal constant. Equation (5.5) now leads to our final result for the correlation length,

$$\xi_+ \sim e^{l^*} = e^{l_1^* + l_2^*} \approx e^{Ct^{-2/5}} \quad (5.22)$$

as  $t \rightarrow 0^+$ , with  $C = C_1 + C_2$ . This prediction should be compared with Kosterlitz' prediction<sup>23</sup> for XY models, which also applies to melting on a square lattice, namely

$$\xi_+ \sim e^{Ct^{-1/2}} \quad (5.23)$$

Since correlations decay as temperature-dependent power laws below  $T_m$ , one could, following Kosterlitz,<sup>23</sup> say that  $\xi_+ = \infty$  everywhere in the crystalline phase. If one instead defines a correlation length in terms of a screening distance associated with dislocation pairs in analogy to recent work by Ambegaokar *et al.*<sup>48</sup> on superfluidity, one finds a correlation length  $\xi_+$  which behaves as  $T \rightarrow T_m^-$  essentially like  $\xi_+$  as  $T \rightarrow T_m^+$

The exponents  $\frac{2}{5}$  and  $\frac{1}{2}$  which enter (5.22) and (5.23) also affect the renormalized elastic constants. In analogy to results for the behavior of the superfluid density  $\rho_s$  as  $T \rightarrow T_c^-$ ,<sup>27</sup> we would expect a  $\frac{2}{5}$ -root cusp singularity in the elastic constants as  $T \rightarrow T_m^-$ , provided one can ignore the

angular terms in the dislocation Hamiltonian discussed in Sec. III A.

#### B. Free energy and specific heat

The transformation law for the reduced free energy per unit area,

$$F(\bar{K}, \bar{y}) \equiv \ln Z_c(\bar{K}, \bar{y})/\Omega, \quad (5.24)$$

which holds for the triangular-lattice renormalization group is

$$F(\bar{K}, \bar{y}) = 6\pi \int_0^1 e^{-2\bar{l}\bar{y}^2(\bar{l})} d\bar{l} + e^{-2\bar{l}} F(\bar{K}(l), \bar{y}(l)). \quad (5.25)$$

The first or "trajectory integral"<sup>49</sup> term in (5.25) comes from the contribution to  $Z_c$  displayed in Eq. (4.25). Evaluating (5.25) at the same value of  $l^*$  as was used for the correlation length we find that

$$F(\bar{K}, \bar{y}) \sim e^{-Bt^{-2/5}} \quad (5.26)$$

as  $T \rightarrow T_m^+$ . The specific heat has the same essential singularity, as can be seen by differentiating (5.26).

#### C. Correlation between Burger's vectors

The scaling law (4.37) for Burger's vector correlations on a triangular lattice can be used to determine their large- $r$  behavior in the crystalline phase. Let us choose  $l = l^*$  in (4.37) such that  $re^{-l^*} = a$ . As  $r \rightarrow \infty$ ,  $l^*$  diverges, and  $\bar{y}(l^*)$  tends to zero. For  $\bar{y}(l^*)$  sufficiently small, we have

$$\Gamma_b(a, \bar{K}(l^*), \bar{y}(l^*)) \approx -6\bar{y}^2(l^*), \quad (5.27)$$

so that

$$\Gamma_b(r, \bar{K}, \bar{y}) = -6\bar{y}^2(l^*) \exp\left(-4l^* - 4\pi \int_0^{l^*} \bar{y}(l) dl\right). \quad (5.28)$$

From (4.36b) it follows that

$$\bar{y}(l) = y_0 \exp\left(2l + 2\pi \int_0^l \bar{y}(l) dl - \frac{1}{8\pi} \int_0^l \bar{K}(\bar{l}) d\bar{l}\right) \quad (5.29)$$

which, when inserted into (5.27), gives

$$\Gamma_b(r, \bar{K}, \bar{y}) = -6y_0^2 \exp\left(-\frac{1}{4\pi} \int_0^{l^*} \bar{K}(\bar{l}) d\bar{l}\right). \quad (5.30)$$

Since  $K(l)$  tends to a constant value as  $l \rightarrow \infty$  for  $T < T_m$ , and because  $l^* = \ln(r/a)$ , we find from (5.30) that

$$\Gamma_b(r, \bar{K}, \bar{y}) \sim (r/a)^{-\bar{K}_{\text{eff}}/4\pi}, \quad (5.31)$$

where  $\bar{K}_{\text{eff}} = \lim_{l \rightarrow \infty} \bar{K}(l)$ .



There are logarithmic corrections<sup>50</sup> to the power-law decay of  $\Gamma_b(r, K, y)$  at  $T_m$ . To leading order in  $x(l)$ , (5.29) may be written

$$\Gamma_b(r, \bar{K}, \bar{y}) = -6y_0^2 \exp\left(-4l^* + 4 \int_0^l x(l) dl\right). \quad (5.32)$$

The logarithmic corrections now follow if we use the result (5.15) for  $x(l)$  along the incoming separatrix, which gives

$$\Gamma_b(r, \bar{K}, \bar{y}) = -6y_0^2 / e^{4l^*} \left(1 + \frac{4}{3} |x_0| l^*\right)^3. \quad (5.33)$$

Thus,

$$\Gamma_b(r, \bar{K}, \bar{y}) \sim 1/r^4 \ln^3 r \quad (5.34)$$

as  $r \rightarrow \infty$  at  $T_m$ . The analogous result for a scalar Coulomb gas is

$$\Gamma_m(r, K, y) \sim 1/r^4 \ln^2 r \quad (5.35)$$

as  $r \rightarrow \infty$  at  $T_c$ .

## VI. REAL MELTING

It is important to determine the relevance of the results presented here to melting of say, rare-gas atoms adsorbed onto a periodic substrate.<sup>51</sup> Such systems might provide an experimental test of the Kosterlitz-Thouless model of melting, some of whose consequences are worked out here. In this concluding section, we raise several issues which affect the applicability of a simple model of dislocation-mediated melting to realistic experimental situations.

It is rather striking that the analysis presented here leads to a second-order phase transition (with a diverging correlation length), contrary to our experience with melting in three dimensions. (Quantities such as the shear modulus can vanish discontinuously at  $T_m$ , however.) This conclusion is based on a perturbative renormalization analysis—an expansion in powers of  $\bar{y}$ , which is only correct at low temperatures or if the core energy of a dislocation is large. Although the results of this paper suggest that an initially large value of  $\bar{y}$  will be driven to zero by the renormalization equations, this can only be checked perturbatively. A first-order transition is not completely ruled out for systems whose dislocations have very small core energies. Holz and Medeiros<sup>52</sup> have recently obtained a first-order transition for a gas of dislocations using a kind of mean-field theory. Their analysis is motivated, however, by an assertion that the “dielastic” polarizability of dislocation dipoles increases with increasing  $T$  until it diverges at  $T_m$ . The results of this paper suggest that this polarizability is per-

fectly finite at all temperatures up to and including  $T_m$ . The finiteness of the polarizability (except above the melting temperature) is due to the extra logarithmic factors in the decay of Burger’s vector correlations at  $T_m$  discussed in Sec. VC.

To apply our results to melting of adsorbed films, one must come to grips with the effects of a periodic substrate potential. This question is discussed in detail in Ref. 28, where it is found that a substrate with a sufficiently small mesh size will have no effect on the melting transition discussed here. Defects and interstitials, which are also a factor in real systems, have in fact already been taken into account. Such imperfections can be regarded as two dislocations one lattice spacing apart, and, as such, are included in the present analysis.

Finally, it should be emphasized that the properties of the dislocation Hamiltonian (2.21) have not yet been completely worked out, since we have neglected the angular terms in  $\mathcal{H}_D$ . Indeed, in Appendix B it is shown that these angular terms represent a *marginal* perturbation to the two-dimensional surface of stable fixed points discussed in this paper. A three-dimensional *volume* of fixed points is necessary to describe the dislocation Hamiltonian in complete generality. Consequently, we would expect some slight qualitative change in the results of Sec. V when these angular terms are taken into account. The relevant calculation is carried out for melting of triangular lattices in Ref. 28; the results confirm this expectation.

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## APPENDIX A: LOCAL REPRESENTATION OF THE DISLOCATION PARTITION SUM

The transformations which led to a local representation of the vector Coulomb-gas partition sum in Sec. III can also be applied to the more-complicated dislocation Hamiltonian (2.21). In Sec. III, we asserted that  $Z_c$  could be approximately represented by

$$Z'_c = \sum_{\{\vec{b}(\vec{r})\}} \int \mathfrak{D}\vec{\phi} \exp\left(-\frac{4\pi^2}{K} \int \frac{d^2r}{a^2} [\vec{\nabla}\vec{\phi}(\vec{r})]^2 + 2\pi i \int \frac{d^2r}{a^2} \vec{b}(\vec{r}) \cdot \vec{\phi}(\vec{r})\right), \quad (\text{A1})$$

which is (3.10a) expressed in a convenient continuum form. On transforming (A1) into momentum space, we shall simulate the effect of a lattice cutoff by restricting the momenta to a circular Brillouin zone of radius  $a^{-1}$ . When we say that  $Z'_c$  "approximates"  $Z_c$ , we mean that the effective interaction between Burger's vectors obtained by integrating out the  $\vec{\phi}$  field in (A1) has the same large-distance form as the Burger's vector interactions in  $\bar{\mathcal{H}}_c$ . If melting is indeed characterized by a diverging correlation length (see Sec. V A), we would expect that only this large-distance behavior would be important in determining the nature of the transition.

To find a local representation of

$$Z_D = \sum_{\{\vec{b}(\vec{r})\}} e^{\bar{\mathcal{H}}_D}, \quad (\text{A2})$$

we consider a generalization of  $Z'_c$  analogous to (3.12), namely,

$$Z'_D = \sum_{\{\vec{b}(\vec{r})\}} \int \mathfrak{D}\vec{\phi} \exp\left(-\frac{1}{2} \int \frac{d^2r}{a^2} \{A[\vec{\nabla}\vec{\phi}(\vec{r})]^2 + B[\vec{\nabla} \cdot \vec{\phi}(\vec{r})]^2\} + 2\pi i \int \frac{d^2r}{a^2} \vec{b}(\vec{r}) \cdot \vec{\phi}(\vec{r}) + \ln y_0 \int \frac{d^2r}{a^2} \vec{b}^2(\vec{r})\right). \quad (\text{A3})$$

The constants  $A$  and  $B$  will be adjusted to make the effective interaction between  $\vec{b}$ 's after eliminating the  $\vec{\phi}$  field as similar as possible to that which occurs in  $\bar{\mathcal{H}}_D$ . Carrying out the Gaussian integrals over  $\vec{\phi}$ , we find

$$Z'_D = Z_0 \sum_{\{\vec{b}(\vec{r})\}} \exp\left(-2\pi^2 \int \frac{d^2r}{a^2} \int \frac{d^2r'}{a^2} b_\alpha(\vec{r}) b_\beta(\vec{r}') \times \langle \phi_\alpha(\vec{r}) \phi_\beta(\vec{r}') \rangle_0\right), \quad (\text{A4})$$

where  $\langle \rangle_0$  means an average evaluated in an ensemble specified by

$$\bar{\mathcal{H}}_c = -\frac{1}{2} \int \frac{d^2r}{a^2} \{A[\vec{\nabla}\vec{\phi}(\vec{r})]^2 + B[\vec{\nabla} \cdot \vec{\phi}(\vec{r})]^2\}, \quad (\text{A5})$$

and

$$Z_0 = \int \mathfrak{D}\vec{\phi} e^{\bar{\mathcal{H}}_c}. \quad (\text{A6})$$

In order that the functional integrals over  $\vec{\phi}$  converge, we must have

$$A > 0, \quad A + B > 0. \quad (\text{A7})$$

It is easy to show that

$$G_{\alpha\beta}(\vec{r}) \equiv \langle \phi_\alpha(\vec{r}) \phi_\beta(\vec{0}) \rangle_0 = \int_q \hat{G}_{\alpha\beta}(\vec{q}) e^{i\vec{q} \cdot \vec{r}}, \quad (\text{A8})$$

where

$$\hat{G}_{\alpha\beta}(\vec{q}) = \frac{1}{Aq^2} \delta_{\alpha\beta} - \frac{B}{A(A+B)} \frac{q_\alpha q_\beta}{q^4} \quad (\text{A9})$$

and  $\int_q$  means  $1/2\pi^2 \int d^2q$ . If this result is inserted into (A4), we clearly obtain a divergent result unless

$$\int d^2r \vec{b}(\vec{r}) = \vec{0}. \quad (\text{A10})$$

Restricting the summation over  $\vec{b}(\vec{r})$  in (A4) to complexions satisfying this condition, we see that  $G_{\alpha\beta}(\vec{r})$  can now be replaced

$$G'_{\alpha\beta}(\vec{r}) = \int_q \hat{G}_{\alpha\beta}(\vec{q}) (e^{i\vec{q} \cdot \vec{r}} - 1). \quad (\text{A11})$$

An analysis of the large- $\vec{r}$  behavior of  $G'_{\alpha\beta}(\vec{r})$  shows that

$$G'_{\alpha\beta}(\vec{r}) = -\frac{1}{4\pi A} \frac{2A+B}{(A+B)} \ln\left(\frac{r}{a}\right) \delta_{\alpha\beta} + \frac{B}{4\pi A(A+B)} \times \frac{r_\alpha r_\beta}{r^2} - C \delta_{\alpha\beta} \quad (\text{A12})$$

where  $C$  is a cutoff-dependent constant. Let us take this as an approximate result for all  $r > a$  and set  $G'_{\alpha\beta}(r) = 0$  for  $r < a$ . Inserting this approximation into (A8) and (A4), we find the  $Z'_D$  becomes

$$Z'_D = Z'_D \propto \sum_{\{\vec{b}(\vec{r})\}} e^{\bar{\mathcal{H}}'_D}, \quad (\text{A13})$$

where the sum over  $\vec{b}(\vec{r})$  is restricted according to (A10), and

$$\bar{\mathcal{H}}'_D = \frac{\pi(2A+B)}{2A(A+B)} \int \frac{d^2r}{a^2} \int_{|\vec{r}-\vec{r}'|>a} \frac{d^2r'}{a^2} \left[ \vec{b}(\vec{r}) \cdot \vec{b}(\vec{r}') \ln\left(\frac{|\vec{r}-\vec{r}'|}{a}\right) \frac{B}{(2A+B)} - \frac{\vec{b}(\vec{r}) \cdot (\vec{r}-\vec{r}') \vec{b}(\vec{r}') \cdot (\vec{r}-\vec{r}')}{|\vec{r}-\vec{r}'|^2} + C \vec{b}(\vec{r}) \cdot \vec{b}(\vec{r}') \right] + \ln y_0 \int \frac{d^2r}{a^2} |\vec{b}(\vec{r})|^2. \quad (\text{A14})$$

Evidently,  $\overline{\mathcal{H}}'_D$  is the same as  $\overline{\mathcal{H}}_D$  in this approximation [see Eq. (2.17)] provided we take

$$\frac{\overline{K}a^2}{8\pi k_B T} = \frac{\pi(2A+B)}{2A(A+B)}, \quad \frac{B}{(2A+B)} = 1. \quad (\text{A15})$$

The coefficient of the term proportional to  $\int (d^2r/a^2)\overline{b}(\vec{r})$  arising from (A14) can be adjusted by changing  $y_0$ .

Unfortunately, we must take  $A=0$  to satisfy the second condition in (A15)! Thus, the most interesting case just violates the stability conditions (A7). One way to sidestep this technical difficulty is to consider (A4) to be a generalization of  $\overline{\mathcal{H}}_D$ . For  $A>0$ , the functional integrals over  $\vec{\phi}$  still converge and we can at least assess the importance of the angular factors in  $\overline{\mathcal{H}}_D$  by perturbation theory in  $B$ . This is done in Appendix B, with the results that they represent *marginal* perturbation to the vector Coulomb-gas partition sum. For  $B=0$ , we obtain the result (3.10).

As is pointed out in Ref. 28, the Hamiltonian (A14) with  $A>0$  is of physical interest in its own right, since it arises in studies of melting on a periodic substrate. With the local representations (A1) and (A3) at hand, one is in a position to study this melting problem using, say, the Migdal-Kadanoff renormalization procedure.

#### APPENDIX B: RENORMALIZATION-GROUP EIGENVALUES FROM THE DECAY OF CORRELATIONS

Given a fixed-point reduced Hamiltonian  $\overline{\mathcal{H}}^*$ , one often wants to determine its stability to small perturbations. Consider, in particular, the Hamiltonian

$$\overline{\mathcal{H}} = \overline{\mathcal{H}}^* + h \int d^2r O(\vec{r}), \quad (\text{B1})$$

where  $h$  measures the strength of the perturbation, and  $O(r)$  is a density constructed from the fluctuating degrees of freedom. At a fixed point, we expect a power-law decay in correlations, and in particular, that

$$C(\vec{r}) = \langle O(\vec{r})O(\vec{0}) \rangle_* \sim r^{-2x_h}, \quad (\text{B2})$$

where the average is evaluated in the fixed-point ensemble. It can be shown<sup>40,50</sup> that the exponent  $x_h$  is related to the renormalization-group eigenvalue  $\lambda_h$  of  $h$  by the formula

$$\lambda_h = d - x_h, \quad (\text{B3})$$

where  $d$  is the dimensionality. The corresponding recursion relation for  $h$  is<sup>40,50</sup>

$$\frac{dh(l)}{dl} = \lambda_h h(l), \quad (\text{B4})$$

so the sign of  $\lambda_h$  determines whether  $h(l)$  grows or shrinks under a renormalization-group transformation.

In this Appendix, we examine the autocorrelations of several important densities  $O(\vec{r})$  which arise in the theory of melting, and thus determine their renormalization group eigenvalues. This procedure was used in Sec. III C to show analytically that  $x = \vec{e}_1 \cdot \vec{e}_2$  represents a marginal perturbation ( $\lambda_x = 0$ ) to the line of fixed points present for  $x=0$ .

We first assess the importance of the periodic part of (3.16). For  $y_0=0$ , we have a Gaussian Hamiltonian which is easily seen to be a fixed point under the renormalization transformations used in this paper,

$$\overline{\mathcal{H}}^* = -\frac{4\pi^2}{K} \sum_{\langle \vec{r}, \vec{r}' \rangle} [\vec{\phi}(\vec{r}) - \vec{\phi}(\vec{r}')]^2. \quad (\text{B5})$$

The density whose correlations determine the eigenvalue  $\lambda_{y_0}$  is

$$O(\vec{r}) = 2\cos[2\pi\vec{e}_a \cdot \vec{\phi}(\vec{r})] + 2\cos[2\pi\vec{e}_b \cdot \vec{\phi}(\vec{r})] + 2\cos[2\pi\vec{e}_c \cdot \vec{\phi}(\vec{r})]. \quad (\text{B6})$$

Since it is easily shown that the autocorrelation of  $O(\vec{r})$  behaves like the autocorrelation of any one term in (B6), we have

$$C(\vec{r}) \sim \langle \cos[2\pi\vec{e}_a \cdot \vec{\phi}(\vec{r})] \cos[2\pi\vec{e}_a \cdot \vec{\phi}(\vec{0})] \rangle \sim \exp[-2\pi^2 e_a^\alpha e_a^\beta \langle \phi_\alpha(\vec{r}) \phi_\beta(\vec{0}) \rangle]. \quad (\text{B7})$$

However,

$$\langle \phi_\alpha(\vec{r}) \phi_\beta(\vec{0}) \rangle \approx \frac{K}{8\pi^3} \ln\left(\frac{r}{a}\right) \delta_{\alpha\beta} \quad (\text{B8})$$

at large  $r$ , so that

$$C(\vec{r}) \sim r^{-\overline{K}/4\pi}. \quad (\text{B9})$$

Thus,  $x_{y_0} = \overline{K}/8\pi$ , and the renormalization-group eigenvalue of  $y$  is

$$\lambda_{y_0} = 2 - \overline{K}/8\pi. \quad (\text{B10})$$

As a second application of this technique, we treat the angular terms in (A3) represented by  $\frac{1}{2}B \int d^2r/a^2 [\vec{\nabla} \cdot \vec{\phi}(\vec{r})]^2$  in the limit of small  $B$ . We assume that the renormalization-group equations have driven  $y_0$  to zero, so that Burger's vector excitations are unimportant. One is left with a fixed point Hamiltonian

$$\overline{\mathcal{H}}^* = -\frac{1}{2}A \int \frac{d^2r}{a^2} [\vec{\nabla} \cdot \vec{\phi}(\vec{r})]^2 \quad (\text{B11})$$

perturbed by a density

$$O(\vec{r}) = -\frac{1}{2}[\vec{\nabla} \cdot \vec{\phi}(\vec{r})]^2. \quad (\text{B12})$$

Although it is evident merely from dimensional

$$C(\vec{r}_1 - \vec{r}_2) \equiv \langle O(\vec{r}_1) O(\vec{r}_2) \rangle = \frac{1}{4} \frac{\partial}{\partial r_{1,\alpha}} \frac{\partial}{\partial r_{1,\beta}} \frac{\partial}{\partial r_{1,\gamma}} \frac{\partial}{\partial r_{1,\delta}} \langle \phi_\alpha(r_1) \phi_\beta(r_1) \phi_\gamma(r_2) \phi_\delta(r_2) \rangle_*. \quad (\text{B13})$$

Since

$$\langle \phi_\alpha(\vec{r}_1) \phi_\beta(\vec{r}_1) \phi_\gamma(\vec{r}_2) \phi_\delta(\vec{r}_2) \rangle_* \sim (\delta_{\alpha\gamma} \delta_{\beta\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma}) \ln^2(|\vec{r}_1 - \vec{r}_2|/a) \quad (\text{B14})$$

at large separations, we find that

$$C(\vec{r}_1 - \vec{r}_2) \equiv |\vec{r}_1 - \vec{r}_2|^{-4} \quad (\text{B15})$$

so that  $x_B = 2$  and  $y_B = 0$ , which are the required results.

*Notes added in proof.* The sign of the angular terms in (2.17) is given incorrectly in many places in the literature, including Ref. 27, Ref. 31, and in F.R.N. Nabarro, *Adv. Phys.* **1** 269 (1952). It is given correctly in Refs. 15 and 32, however. I

analysis that (B12) must represent a marginal perturbation to (B11), it is interesting to see how this result follows from the decay of  $O(r)$  correlations. The relevant correlation function is

am indebted to A. P. Young for discussions on this point.

The exact nature of the cancellations between different complexions of Burger's vectors shown in Figs. 5(c) and 7(c) is quite subtle. As was pointed out to me by T. Spencer, it is difficult to show that such configurations are indeed negligible for below  $T_m$ , although this is certainly expected on physical grounds. Such considerations have no effect on our analysis of dislocation unbinding near  $T_m$ , however.

As is shown in Ref. 28, the "fluid" phase discussed in this paper (corresponding to the region of instability in Fig. 6) is actually a bizarre kind of liquid crystal. A second *disclination* unbinding transition is necessary to complete the transition from a crystalline solid into an isotropic liquid.<sup>28</sup>

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$$\epsilon_{ij} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

We shall often make use of the identity  $\epsilon_{ij}\epsilon_{jk} = -\delta_{ik}$ .

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<sup>38</sup>The Poisson summation formula asserts that the sum over discrete states  $p$  of any function  $g(p)$  may be written

$$\sum_{p=-\infty}^{\infty} g(p) = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} dP g(P) e^{2\pi imP}.$$

<sup>39</sup>See, e.g., S. Coleman, *Phys. Rev. D* 11, 2088 (1972); A. Luther and I. Peschel, *Phys. Rev. B* 9, 2911 (1974).

<sup>40</sup>See, e.g., L. P. Kadanoff in *Proceedings of the Enrico Fermi Summer School of Physics, Varenna*, 1970, edited by M. S. Green (Academic, New York, 1971); and K. J. Wilson and J. Kogut, *Phys. Rep. C* 12, 77 (1974).

<sup>41</sup>P. G. DeGennes, *Solid State Commun.* 10, 753 (1972).

<sup>42</sup>W. L. McMillan, *Phys. Rev. A* 6, 936 (1972); 7, 1673 (1973).

<sup>43</sup>See, e.g., R. A. Pelcovits, Ph.D. thesis (Harvard University, 1978) (unpublished).

<sup>44</sup>See also, J. Villain, *J. Phys. (Paris)* 36, 581 (1975).

<sup>45</sup>See, e.g., V. J. Emery and R. H. Swendsen, *Phys. Rev. Lett.* 39, 1414 (1977), *Phys. Lett. A* 64, 325 (1977). See also A. N. Berker, S. Ostlund, and E. Putnam, *Phys. Rev. B* (to be published).

<sup>46</sup>L. P. Kadanoff and F. J. Wegner, *Phys. Rev. B* 4, 3987 (1971).

<sup>47</sup>R. J. Baxter, *Phys. Rev. Lett.* 26, 832 (1971).

<sup>48</sup>V. Ambegaokar, B. I. Halperin, D. R. Nelson, and E. D. Siggia, *Phys. Rev. Lett.* 40, 783 (1978).

<sup>49</sup>See, e.g., D. R. Nelson, *Phys. Rev. B* 11, 3504 (1975).

<sup>50</sup>*Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 6.

<sup>51</sup>J. G. Dash, *Films on Solid Surfaces* (Academic, New York, 1975).

<sup>52</sup>A. Holz and J. T. N. Medeiros, *Phys. Rev. B* 17, 1161 (1978).