Dislocation-disclination melting of two-dimensional lattices

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The melting of two-dimensional lattices is analyzed in the mean-field approximation. The model used here incorporates long-wavelength fluctuations of the one-particle distribution function and also orientation fluctuations of the two-particle distribution function. The nature of the transition depends on the intensity of orientation fluctuations (α), the energy of the disclination core (E_c), and the relative size of this core (t). Above a critical value α_c, the system melts through two continuous transitions. In the first transition, dislocation pairs undergo dissociation, and a hexatic phase forms. In the second transition, this hexatic phase becomes an ordinary liquid through a dissociation of the disclination pairs. The universal relation $a_0^2 n_0(T_i) = \pi/108$ holds on the line of the latter transition, where $n_0(T_i)$ is the density of free dislocations. Under the condition $\alpha < \alpha_c$, the system melts through two continuous transitions if the energy of the disclination core is above a critical value E_c^*. If the condition $E_c < E_c^*$ holds instead, the system melts through a single first-order transition, in the course of which the disclination complexes dissociate. The parameters of the first-order transition depend on E_c, t, and α.

INTRODUCTION

The nature of melting in a two-dimensional situation has recently been the subject of a lively discussion. Halperin, Nelson, and Young[2–5] have generalized a well-known study by Kosterlitz and Thouless[1] and have shown that a possible scenario for the melting of two-dimensional lattices might be fundamentally different from that in the case of three dimensions: The lattice would melt through two continuous transitions. In the course of the first transition, dislocation pairs would dissociate; in the second transition, disclination pairs would dissociate. That analysis was carried out on the basis of classical elastic theory under the assumption that the dislocation cores have a high energy. The theory of dislocation melting has found support in several experiments and also in the results of numerical simulations of certain two-dimensional systems.[6–11]

There are, on the other hand, theories[12,13] which show that melting occurs through a first-order transition, as in the case of three dimensions. These theories agree with many numerical simulations (Refs. 14–16, for example).

Noteworthy in this connection is the study by Dimon *et al.*,[17] who showed, in research on the melting of xenon adsorbed on graphite, that the melting proceeds as a first-order transition at low temperatures and densities, while at high values of these properties it proceeds continuously.

A numerical simulation has revealed the important role played by the energy of the dislocation core:[7,18] At low energies, one would expect a first-order transition, while at high energies one would expect a continuous transition (or something close to it).[13]

The difficulties here are difficult to resolve on the basis of theories grounded in standard elastic theory.[19] Our purpose in the present paper is to analyze the melting of two-dimensional lattices on the basis of a model which incorporates not only long-wavelength fluctuations of the one-particle distribution function (and which in this regard is equivalent to standard elastic theory) but also orientation fluctuations of the two-particle distribution function.

DISLOCATION–DISCLINATION HAMILTONIAN

A crystal differs from an isotropic liquid in that two symmetries are broken: translational and rotational. These two symmetries are not independent, since a rotation of one part of an ideal crystal with respect to another part disrupts not only the orientational order but also the translational order. In an ideal crystal a one-particle distribution function has the symmetry of the crystal lattice. One can, on the other hand, imagine a state of a condensed medium in which there is no translational long-range order (i.e., in which the one-particle distribution function is constant) but in which there are long-range correlations between the directions of the "bonds," where a "bond" is to be understood as a vector which connects two nearest neighbors.[20] In this case the isotropy of the two-particle distribution function, which characterizes the relative spatial distribution of pairs of particles, is disrupted.[21]

It is well known that in two dimensions the long-range translational order is disrupted by fluctuations, although at low temperatures there is a slow, power-law decay of correlations.[22,23] On the other hand, it follows from Ref. 24 (see also Ref. 4) that a state with an orientational long-range order, characterized by a disruption of the isotropy of the two-particle distribution function, can exist in two dimensions.

At sufficiently low temperatures, the local density, proportional to the one-particle distribution function, can be expanded in a Fourier series in reciprocal-lattice vectors $\{\mathbf{G}\}$:

$$\rho(\mathbf{r}) = \sum \rho_{\mathbf{G}}(\mathbf{r}) e^{i\mathbf{G}\mathbf{r}},$$

where the Fourier coefficients $\rho_{\mathbf{G}}(\mathbf{r})$ vary slowly over distances on the order of G^{-1} and have the amplitude and the phase

$$\rho_{\mathbf{G}}(\mathbf{r}) = |\rho_{\mathbf{G}}(\mathbf{r})| e^{i\mathbf{G}\mathbf{u}(\mathbf{r})}.$$

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Here $\mathbf{u}(\mathbf{r})$ is the displacement field. In two dimensions, the phase of the order parameter fluctuates the most,[23] so we will ignore fluctuations in the magnitude.

In general, the one-particle and two-particle distribution functions are not independent, but the two-particle distribution function may have an anisotropic part which does not vanish even in the case $\rho(\mathbf{r}) = \text{const}$. This quantity describes a state with an orientational ordering of bonds.[20,21] The probability for finding a particle at the point $\mathbf{r}$ under the condition that another particle is pinned at the point $\mathbf{r}_0$ is characterized by the conditional two-particle distribution function $F_2(\mathbf{r}|\mathbf{r}_0)$:

$$F_2(\mathbf{r}|\mathbf{r}_0)=F_2(\mathbf{r},\ \mathbf{r}_0)/F_1(\mathbf{r}_0),$$

where $F_2(\mathbf{r},\mathbf{r}_0)$ is the two-particle distribution function, and $F_1(\mathbf{r}_0)$ the one-particle distribution function. In a homogeneous and isotropic liquid we would have $F_1(\mathbf{r})\equiv 1$ and $F_2(\mathbf{r},\mathbf{r}_0)=g(|\mathbf{r}-\mathbf{r}_0|)$. Here $g(\mathbf{r})$ is the radial distribution function of the liquid. Let us assume that $\mathbf{r}$ and $\mathbf{r}_0$ are nearest neighbors: $\mathbf{r}-\mathbf{r}_0=\mathbf{a}_0$. When long-range correlations in the direction of the "bonds" $\mathbf{a}_0$ arise, the isotropy of the two-particle distribution function $F_2(\mathbf{r},\mathbf{r}_0)$ is then disrupted. We denote the anisotropic part of the function $F_2(\mathbf{r}|\mathbf{r}_0)$ by $f(\mathbf{r}|\mathbf{r}_0)$. The function $f(\mathbf{r}|\mathbf{r}_0)$ has the symmetry of the local surroundings of the molecule $\mathbf{r}_0$. In the case of two dimensions, this function is

$$f(\mathbf{r}|\mathbf{r}_0)=f(a_0,\ \mathbf{r}_0,\ \varphi),$$

where the angle φ specifies the direction of the vector $\mathbf{a}_0$. The function $f(a_0,\mathbf{r}_0,\varphi)$ can be expanded in a Fourier series:

$$f(a_0,\mathbf{r}_0,\varphi)=\sum_{m=-\infty}^{\infty} f_m(a_0,\mathbf{r}_0)e^{im\varphi}.$$

The Fourier coefficients $f_m(a_0,\mathbf{r}_0)$ are the order parameters of the anisotropic phase. They vary slowly with $\mathbf{r}_0$ and have the amplitude and phase

$$f_m(a_0,\ \mathbf{r}_0)=|f_m(a_0,\ \mathbf{r}_0)|\exp[im\omega(\mathbf{r}_0)].$$

As in the case of the one-particle distribution function, we consider fluctuations in the phase alone.

The free energy of the system is a functional of $\rho(\mathbf{r})$ and $f(\mathbf{r}|\mathbf{r}_0)$. Taking account of the slow variation in the functions $\mathbf{u}(\mathbf{r})$ and $\omega(\mathbf{r})$, we write the thermodynamic potential (Hamiltonian) describing the fluctuations of the order parameter in the two-dimensional system for a triangular lattice as the following expansion:

$$F=\frac{1}{2}\int d^2r[\mu(\partial_i u_j)^2+(\mu+\lambda)(\partial_i u_i)^2]$$
$$+2\alpha\int d^2r(\partial_i\omega)^2=F_1+F_2. \qquad (1)$$

Here $\partial_i=\partial/\partial r_i$, and a repeated index in (1) implies a summation. Assuming periodic boundary conditions, and integrating by parts, we can put F_1 in the standard form of the free energy of a deformed isotropic solid. In this case μ and λ are Lamé coefficients.[19] All previous theories[1-5,7,13,25] of melting have considered the term F_1 alone.

The angle $\omega(\mathbf{r})$ in (1) describes the fluctuations in the directions of the bonds associated with a particle at the point $\mathbf{r}$. In the continuum approximation this angle is related to the displacement field $\mathbf{u}(\mathbf{r})$ by[26]

$$\omega(\mathbf{r})={}^1/_2\varepsilon_{ij}\partial_i u_j(\mathbf{r}), \qquad (2)$$

where ε_{ij} is the antisymmetric matrix:

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

Substituting (2) into (1), we find a Hamiltonian which we will use to describe the two-dimensional melting:

$$F=\frac{1}{2}\int d^2r[\mu(\partial_i u_j)^2+(\mu+\lambda)(\partial_i u_i)^2]$$
$$+\frac{\alpha}{2}\int d^2r\varepsilon_{ij}\varepsilon_{lm}\partial_i\partial_k u_j\partial_l\partial_k u_m. \qquad (3)$$

In a two-dimensional system with continuous symmetry, a phase transition is known to be caused by the appearance of topological singularities: vortices which disrupt the quasi-long-range order.[1,23] In a two-dimensional crystal there are two types of such defects: dislocations and disclinations. Dislocations can be thought of as disclination dipoles.[5,7,26] Kosterlitz and Thouless[1] showed that the appearance of free dislocations leads to a melting of a two-dimensional lattice to form a liquid which is characterized by a density-density correlation function which falls off exponentially with distance (in contrast with the power-law decay of this function in a two-dimensional crystal). The phase which forms in the case of the dislocation melting, however, is characterized by a power-law decay of the correlations between the directions of the bonds,[2,4] although the magnitude of the displacement $\mathbf{u}$ of this phase is zero. This phase has been called a "hexatic" phase.[2,4] The hexatic phase becomes an ordinary liquid through a dissociation of disclination pairs accompanied by the formation of free disclinations at a temperature above the dislocation-melting point.

One can, on the other hand, picture the melting as occurring as a single transition rather than a two-step process. In this single transition, free disclinations arise immediately, and there is no hexatic phase.

Let us consider two melting scenarios on the basis of Hamiltonian (3). For this purpose we distinguish the part of (3) which corresponds to the ensemble of dislocations and disclinations. Hamiltonian (3) can be rewritten as

$$F=\frac{1}{2}\int d^2r[2\mu u_{ij}^2+\lambda u_{kk}^2]+2\alpha\int d^2r\varepsilon_{ij}\varepsilon_{lm}\partial_i u_{jk}\partial_l u_{mk}, \qquad (4)$$

where $u_{ij}=\frac{1}{2}[\partial_i u_j(\mathbf{r})+\partial_j u_i(\mathbf{r})]$ is the strain tensor. In deriving (4) we used the relation

$$\partial_k\omega=\varepsilon_{ij}\partial_i u_{jk}. \qquad (5)$$

To find an explicit expression for the part of the free energy due to dislocations and disclinations, we write the strain tensor in the form

$$u_{ij}=\Phi_{ij}+u_{ij}^s, \qquad (6)$$

where Φ_{ij} is the strain tensor generated by regular strains $\Phi_i(\mathbf{r})$, and u_{ij}^s reflects the contribution of disclinations and dislocations to the strain tensor.

A dislocation at the point $\mathbf{r}$ is characterized by the size of the increment in the contour integral of the displacement field when a closed loop is traced out around the dislocation:[19]

$$\oint d\mathbf{u}=-a_0\mathbf{b}(\mathbf{r})=-n(\mathbf{r})a_0\mathbf{e}_1-m(\mathbf{r})a_0\mathbf{e}_2, \qquad (7)$$

where $\mathbf{b}(\mathbf{r})$ is the dimensionless Burgers vector, a_0 is the period of the triangular lattice, $\mathbf{e}_1$ and $\mathbf{e}_2$ are basis vectors of the lattice, and m and n are integers.

Correspondingly, a disclination on a triangular lattice is characterized by the circumstance that when a closed loop containing the disclination is traced out the integral of the rotation angle (2) acquires an increment which is a multiple of $2\pi/6$:

$$\oint d\omega(\mathbf{r}) = -(2\pi/6)s, \quad s = \pm 1, \pm 2, \ldots . \tag{8}$$

[The contours in (7) and (8) are traversed in the counterclockwise direction.]

We find equations for the field $\mathbf{u}(\mathbf{r})$ from (3):

$$\frac{\delta F}{\delta u_p} = -(\mu+\lambda)\partial_p\partial_l u_l - \mu\nabla^2 u_p - \alpha\nabla^2\varepsilon_{pl}\partial_l\omega = 0.$$

This equation can be rewritten in the form

$$\sigma_{ij} = 2\hat{\mu}u_{ij} + \hat{\lambda}u_{ll}\delta_{ij}, \qquad 2\hat{\mu} = 2\mu - \alpha\nabla^2, \quad \hat{\lambda} = \lambda + \alpha\nabla^2. \tag{9}$$

where the tensor σ_{ij} is given by

$$\partial_j\sigma_{ij} = 0, \tag{10}$$

Equation (9) has the form of the equilibrium equation of a deformed object, and the symmetric tensor σ_{ij} is the stress tensor. The tensor σ_{ij} takes the standard form[19] when we allow for the conversion of the Lamé coefficients μ and λ into operators $\hat{\mu}$ and $\hat{\lambda}$.

Using (6) and (10), we can decompose the tensor σ_{ij} into regular and singular parts. We write u_{ij}^s in terms of the singular part of the stress tensor, σ_{ij}^s. Using (10), we find

$$u_{ij}{}^s = \frac{\sigma_{ij}{}^s}{2\hat{\mu}} - \frac{\hat{\lambda}}{4\hat{\mu}(\hat{\mu}+\hat{\lambda})}\sigma_{ll}{}^s\delta_{ij}. \tag{11}$$

The stress tensor can be written in terms of the stress function[19,26] $\chi(\mathbf{r})$:

$$\sigma_{ij}{}^s = \varepsilon_{ik}\varepsilon_{jl}\partial_k\partial_l\chi(\mathbf{r}). \tag{12}$$

Using Green's formula, we find from (7) and (8) equations for u_{ij}^s for a dislocation at the point $\mathbf{r}'$ and for a disclination at the point $\mathbf{r}''$, respectively:

$$\varepsilon_{ij}\varepsilon_{mn}\partial_i\partial_m u_{jn}{}^s = -a_0\varepsilon_{mn}\partial_m b_n\delta(\mathbf{r}-\mathbf{r}'), \tag{13}$$

$$\varepsilon_{ij}\partial_i\partial_j\omega = \varepsilon_{ij}\varepsilon_{lm}\partial_i\partial_l u_{mj}{}^s = -(2\pi/6)s\delta(\mathbf{r}-\mathbf{r}''). \tag{14}$$

Using these equations along with (11) and (12), we find an equation for $\chi(\mathbf{r})$ under the condition that there are N disclinations at the points $\mathbf{r}_j$ and M dislocations at the points $\mathbf{r}_i$:

$$\nabla^4\chi(\mathbf{r}) = -\frac{4\hat{\mu}(\hat{\mu}+\hat{\lambda})}{2\hat{\mu}+\hat{\lambda}}\left\{\sum_{j=1}^{N}\frac{\pi}{3}s_j\delta(\mathbf{r}-\mathbf{r}_j) + a_0\sum_{i=1}^{M}\varepsilon_{mn}\partial_m b_n(\mathbf{r}_i)\delta(\mathbf{r}-\mathbf{r}_i)\right\}. \tag{15}$$

A solution of Eq. (15) is

$$\chi(\mathbf{r}) = -\frac{\mu(\mu+\lambda)}{6(2\mu+\lambda)}\sum_{j=1}^{N}s_j|\mathbf{r}-\mathbf{r}_j|^2\ln\frac{|\mathbf{r}-\mathbf{r}_j|}{a} + \frac{\alpha\lambda}{3(2\mu+\lambda)}\sum_{j=1}^{N}s_j\ln\frac{|\mathbf{r}-\mathbf{r}_j|}{a}$$

$$-\frac{a_0}{4\pi}\frac{4\mu(\mu+\lambda)}{2\mu+\lambda}\sum_{i=1}^{M}\varepsilon_{mn}b_n(\mathbf{r}_i)(\mathbf{r}-\mathbf{r}_i)_m\left[\ln\frac{|\mathbf{r}-\mathbf{r}_i|}{a}+C\right]+\vartheta(\mathbf{r}) \tag{16}$$

where a and C are constants, and $\vartheta(\mathbf{r})$ is a singular function which contains a δ-function and its first derivative. This part generates a short-range interaction of disclinations and dislocations with each other. The short-range part does not lead to the formation of bound states, so we will consider this term no further.

Substituting (6) into (4), we find for F the representation

$$F = F^r + F^s,$$

where F^r corresponds to the regular part of the strain tensor, and F^s corresponds to the singular part, which is generated by the dislocations and disclinations (one can show that the cross terms vanish). Substituting (11) and (12) into (4), we find the singular part of the free energy in terms of the stress function $\chi(\mathbf{r})$:

$$F^s = \int d^2r\{\hat{\Psi}\chi(\mathbf{r})\}\nabla^4\chi(\mathbf{r}), \qquad \hat{\Psi} = \frac{1}{2}\frac{\hat{\mu}^2+\mu\hat{\lambda}-\alpha(2\mu+\lambda)\nabla^2}{\hat{\mu}(\hat{\mu}+\hat{\lambda})}. \tag{17}$$

Substituting (15) and (16) into (17), we find the energy of the system of dislocations and disclinations:

$$F = \frac{\pi}{18}\sum_{i\neq j}^{N}s_is_j\left\{\frac{K}{8}r_{ij}^2\ln\frac{r_{ij}}{a} - 2\alpha\ln\frac{r_{ij}}{a}\right\} + E_c\sum_{j=1}^{N}s_i^2 + \frac{Ka_0}{12}\sum_{i=1}^{M}\sum_{j=1}^{N}s_j\varepsilon_{mn}b_n(\mathbf{r}_i)(\mathbf{r}_j-\mathbf{r}_i)_m\left(\ln\frac{r_{ij}}{a}+C\right) + E_d\sum_{i=1}^{M}\mathbf{b}^2(\mathbf{r}_i)$$

$$-\frac{a_0^2K}{8\pi}\sum_{i\neq j}^{M}\left\{\mathbf{b}(\mathbf{r}_i)\mathbf{b}(\mathbf{r}_j)\ln\frac{r_{ij}}{a} - \frac{(\mathbf{b}(\mathbf{r}_i)\mathbf{r}_{ij})(\mathbf{b}(\mathbf{r}_j)\mathbf{r}_{ij})}{r_{ij}^2}\right\}, \tag{18}$$

where E_c and E_d are the energies of the disclination cores and dislocation cores, respectively,

$$\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j, \quad K = 4\mu(\mu+\lambda)/(2\mu+\lambda).$$

The first two terms describe the energy of the interacting dislocations, while the third describes the interaction of dislocations with disclinations. The last two terms describe the interaction energy of dislocations. It can be shown that the energy of a given configuration of disclination and dislocation charges is finite only under the conditions

$$\sum_j s_j = 0, \quad \sum_j \mathbf{r}_j s_j = 0; \quad \sum_i \mathbf{b}(\mathbf{r}_i) = 0. \tag{19}$$

The last term in Hamiltonian (3) does not contribute to the long-range interaction between dislocations (although it does contribute to E_d). It is not difficult to see that the interaction between dislocations is the same as the dipole–dipole disclination interaction (the Burgers vector $\mathbf{b}$ is orthogonal to the disclination dipole moment vector $\mathbf{d}$: $d_1 = b_2$, $d_2 = -b_1$, $d^2 = b^2$). As we know,[5,7,26] a dislocation may

be thought of as a disclination dipole, so we will use the dipole moment **d** instead of the Burgers vector **b** in the discussion below. Conditions (19) show that there are no free disclinations or disclination dipoles (i.e., dislocations) in a two-dimensional lattice.

MELTING OF TWO-DIMENSIONAL LATTICES

In the low-temperature phase, dislocations can exist only as pairs with a zero Burgers vector, while disclinations can exist as strongly coupled quadrupole complexes. As the temperature is raised, free dislocations may arise, or free disclinations may arise at once, according to the melting scenarios outlined above. In the former case, the free dislocation charges screen the charges of opposite sign, leading to a short-range (exponentially decaying) interaction between dislocations. The interaction between disclinations is modified; while remaining a long-range interaction, it increases only as $\ln r$. The system converts into an ordinary liquid after the appearance of free disclinations. In the latter case, the system becomes a liquid through one transition. As a result of the screening, the interaction between disclinations becomes a short-range interaction.

To describe the dislocation-disclination melting, we use a method similar to the well-known Debye-Hückel method in plasma theory. The energy required for the formation of a disclination or a dislocation depends on the magnitude of the disclination charge, s, or that of the Burgers vector **b**. We consider defects with the lowest energy, namely, disclinations with $s = \pm 1$ and single dislocations on a triangular lattice:

$$\mathbf{d}^1=\begin{pmatrix}3^{1/2}/2\\ 1/2\end{pmatrix},\quad \mathbf{d}^2=\begin{pmatrix}3^{1/2}/2\\ -1/2\end{pmatrix},\quad \mathbf{d}^3=\begin{pmatrix}0\\ -1\end{pmatrix},$$

$$\mathbf{d}^4=\begin{pmatrix}-3^{1/2}/2\\ -1/2\end{pmatrix},\quad \mathbf{d}^5=\begin{pmatrix}-3^{1/2}/2\\ 1/2\end{pmatrix}\quad \mathbf{d}^6=\begin{pmatrix}0\\ 1\end{pmatrix}.$$

We see that Eq. (15) is analogous to the Poisson equation in electrostatics, with the function $\chi(\mathbf{r})$ serving as electrostatic potential. Substituting (15) into (17), and using $\varepsilon_{mn}\partial_n b_m = \partial_m d_m$, we find

$$F^*=U_1+U_2,$$

where

$$U_1=-\frac{\pi}{3}\sum_{j=1}^{N} s_j\hat{\Psi}\chi(\mathbf{r}_j), \tag{20}$$

$$U_2=\sum_{i=1}^{M} a_0 d_m(\mathbf{r}_i)\,\hat{\Psi}\partial_m\chi(\mathbf{r}_i), \tag{21}$$

Here U_1 is the energy of the system of N disclinations in the potential $\chi(\mathbf{r})$, and U_2 is the energy of the M dislocations. Assuming that the dislocation density $n(\mathbf{r})$ and the disclination density $m(\mathbf{r})$ are small, we can use the Boltzmann relation for the density of defects in the field $\chi(\mathbf{r})$:

$$n^i(\mathbf{r})=n_0\exp\{-a_0\beta d_m{}^i\hat{\Psi}\partial_m\chi(\mathbf{r})\}, \tag{22}$$

$$m(\mathbf{r})=m_0\exp\{(\pi/3)\beta s\hat{\Psi}\chi(\mathbf{r})\}. \tag{23}$$

Here $\beta = 1/k_B T$, and k_B is the Boltzmann constant (in the discussion below, k_B will be included in the definition of the temperature). In deriving (22) and (23) we used (20) and (21). Let us use Eqs. (22) and (23) to describe the screening of dislocations and disclinations [the presence of six types of elementary dislocations on a triangular lattice has been taken into account explicitly in Eq. (22)].

The equation for the stress function $\chi(\mathbf{r})$ in the case in which a dislocation $\mathbf{d}^i$ at the point $\mathbf{r}'$ is screened by dislocations and disclinations is

$$\nabla^4\chi(\mathbf{r})=-\frac{4\hat{\mu}(\hat{\mu}+\hat{\lambda})}{2\hat{\mu}+\hat{\lambda}}\Big\{a_0 d_m{}^i\partial_m\delta(\mathbf{r}-\mathbf{r}')+a_0\sum_{i=1}^{6} d_m{}^i\partial_m n_i(\mathbf{r})$$
$$+(\pi/3)m^+(\mathbf{r})-(\pi/3)m^-(\mathbf{r})\Big\}. \tag{24}$$

Here $n_i(\mathbf{r})$ is given by Eq. (22), and m^+ and m^- are found from (23) by setting $s = 1$ and $s = -1$. A corresponding equation for the screening of a disclination with $s = 1$ is found from (24) by replacing the first term on the right-hand side by $(\pi/3)\delta(\mathbf{r}-\mathbf{r}')$. Equation (24) corresponds to the Poisson-Boltzmann equation in Debye-Hückel theory.

We now linearize the right-hand side of Eq. (24) with respect to $\chi(\mathbf{r})$ and take Fourier transforms:

$$\chi(\mathbf{r})=\frac{1}{(2\pi)^2}\int d^2k\, e^{i\mathbf{k}\mathbf{r}}\chi(\mathbf{k}).$$

A solution of this equation is

$$\chi(\mathbf{k})=-\frac{a_0[4\mu(\mu+\lambda)+2\alpha\lambda k^2-\alpha k^4]\,id_m{}^i k_m e^{-i\mathbf{k}\mathbf{r}'}}{(2\mu+\lambda)A(k)},$$

$$A(k)=b_6 n_0 k^6+(1+b_4 n_0+c_4 m_0)k^4+(b_2 n_0+c_2 m_0)k^2+c_0 m_0,$$

$$b_6=3\alpha^2\beta a_0{}^2/2(2\mu+\lambda),\quad b_4=6\alpha\beta a_0{}^2,\quad c_4=\pi^2\alpha^2\beta/9(2\mu+\lambda),$$
$$b_2=24\beta a_0{}^2 K,\quad c_2=4\pi^2\alpha\beta/9,\quad c_0=\pi^2\beta K/9.$$

The solution for the screening of a disclination can evidently be found by replacing $id_m k_m$ by $(\pi/3)s$.

As was mentioned above, melting may be thought of as the appearance of nonzero densities m_0 and n_0. Our problem is to construct closed equations for these quantities. We assume that the gas of dislocations and disclinations is of low density. We can then write the following expressions for n_0 and m_0 with the help of Boltzmann relations:

$$m_0=(1/\Delta)\exp(\beta\mu_1), \tag{25}$$

$$n_0=(1/\Delta)\exp(\beta\mu_2), \tag{26}$$

where μ_1 and μ_2 are the chemical potentials of the disclinations and dislocations, respectively, and the dimensional factor Δ is equal to the area of the unit cell of the lattice and is given by

$$\Delta=a_0{}^2\cdot 3^{1/2}/2.$$

The chemical potential of a disclination consists of two parts: the energy of the disclination core, E_c (this energy incorporates nonlinear effects), and the elastic energy of an individual disclination, $\tilde{U}_1$:

$$\mu_1=-(E_c+\tilde{U}_1). \tag{27}$$

Correspondingly, for a dislocation we write

$$\mu_2 = -(E_d + \tilde{U}_2) \tag{28}$$

(the quantities $\tilde{U}_1$ and $\tilde{U}_2$ are analogous to the self-energy of a charge in electrostatics). To calculate U_1 and U_2, we use (20) and (21). As in electrostatics, these quantities diverge in the case of point charges. Dislocations and disclinations have finite dimensions (r_0' and r_0, respectively), so we can write the estimates $\tilde{U}_1 \approx U_1(r_0)$ and $\tilde{U}_2 \approx U_2(r_0')$ of the self-energies of a disclination and a dislocation. Taking Fourier transforms of (20) and (21) [using (17)], and substituting in the expression for $\chi(\mathbf{k})$, we find

$$U_1(r_0) = \frac{1}{18(2\mu+\lambda)} \times \int d^2k \frac{\mu(\mu+\lambda)+\alpha(2\mu+\lambda)k^2+\alpha^2k^4/4}{A(k)} \exp(i\mathbf{k}\mathbf{r}_0), \tag{29}$$

$$U_2(r_0') = \frac{a_0^2}{(2\pi)^2(2\mu+\lambda)} \int d^2k \frac{k^2[\mu(\mu+\lambda)+\alpha(2\mu+\lambda)k^2+\alpha^2k^4/4]}{A(k)} \times \exp(i\mathbf{k}\mathbf{r}_0'). \tag{30}$$

Equations (25)–(30) constitute a closed system of equations for determining m_0 and n_0 (the densities of free disclinations and dislocations). This system has a solution $m_0 = n_0 = 0$, which corresponds to an "unmelted" crystal. A general analysis of Eqs. (25)–(30) is rather complicated, so we turn to the most important particular cases.

1. Dislocation melting. We first consider the melting of a two-dimensional crystal through the formation of free dislocations.[1-5,25] This case corresponds to $m_0 = 0$. We evaluate the integral in (30) in the approximation $n_0 \ll 1$ [in agreement with (26)]:

$$U_2(r_0') \approx (a_0^2/8\pi) K K_0[r_0'(b_2 n_0/2)^{1/2}], \tag{31}$$

where $K_0(x)$ is a modified Bessel function. We introduce the screening radius

$$\xi' = (b_2 n_0/2)^{-1/2}.$$

It can be seen from (31) that when there are free dislocations the interaction between dislocations has a behavior $\exp(-r/\xi')$. At $r_0'/\xi' \ll 1$ we have

$$U_2(r_0') \approx (a_0^2/8\pi) K[C + \ln(r_0'/2\xi')], \tag{32}$$

where C is Euler's constant. Substituting (32) into (27) and (26), we find an equation for ξ':

$$\left(\frac{r_0'}{\xi'}\right)^2 = q\left(\frac{r_0'}{\xi'}\right)^{a_0^2 K/8\pi T}, \tag{33}$$

where

$$q = \frac{t'^2 b_2}{3^{1/2}} \exp\left[\frac{a_0^2 K}{8\pi T}(C - \ln 2)\right] \exp\left(-\frac{E_d}{T}\right), \quad t' = \frac{r_0'}{a_0}.$$

We obviously have $q < 1$ for sufficiently large values of E_d. In this case we see from Eq. (33) that for $T < T_c = Ka_0^2/16\pi$ we have the unique solution $r_0'/\xi' = 0$, which corresponds to a crystalline phase. At $T > T_c$ we have

$$\frac{r_0'}{\xi'} = q^z, \quad z = \left(2 - \frac{Ka_0^2}{8\pi T}\right)^{-1}.$$

The dislocation melting thus occurs at

$$T_c = Ka_0^2/16\pi. \tag{34}$$

The transition temperature is the same as that found in Refs. 1–5 and 25.

2. Hexatic phase. As was pointed out in Ref. 4, as a result of dislocation melting the system goes into a state with a slow decay of the correlations along the directions of the bonds. In other words, the relation

$$\langle e^{-i\theta_\omega(\mathbf{r})} e^{i\theta_\omega(0)} \rangle \propto r^{-\eta(T)}. \tag{35}$$

holds. This state, called the "hexatic phase" in Ref. 4, becomes an ordinary liquid through a Kosterlitz–Thouless transition, in the course of which disclination pairs undergo dissociation. The phenomenological Hamiltonian

$$H_A = \frac{1}{2} K_A(T) \int d^2r [\nabla\omega(\mathbf{r})]^2, \tag{36}$$

was proposed in Ref. 4 for describing the hexatic phase; the quantity $K_A(T)$ can be called a "Frank modulus" by analogy with liquid crystals. Standard calculations[4,23,28] lead to

$$\eta(T) = 18T/\pi K_A(T).$$

A Kosterlitz–Thouless transition occurs at the temperature T_i such that $\eta(T_i) = \frac{1}{4}$; i.e.,

$$T_i = \pi K_A(T_i)/72. \tag{37}$$

Halperin and Nelson[4] showed that in the hexatic phase the Lamé coefficients renormalized by free dislocations, μ_R and λ_R, vanish. Making use of that circumstance, we find from (25), (28), and (29) an equation for determining the screening radius of free disclination charges:

$$(r_0/\xi)^2 = q'(r_0/\xi)^{z'}, \quad z' = \pi/54a_0^2 n_0(T), \tag{38}$$

where

$$\xi^{-1} = \frac{1}{2}\left[\frac{2\pi^2 m_0}{27a_0^2 n_0(T)}\right]^{1/2}, \quad q' = \frac{t^2\pi^2}{3^{1/2}a_0^2 n_0(T)} \exp\left(-\frac{E_c}{T}\right),$$

$$t = \frac{r_0}{a_0}.$$

At large energies of the disclination core we have $q' < 1$. In this case, Eq. (38) has a nontrivial solution under the condition

$$a_0^2 n_0(T) \geqslant \pi/108. \tag{39}$$

Expression (39) with the equal sign gives the density of dislocations on the (hexatic phase)–(ordinary liquid) transition line. Comparing (37) with (39), we find expressions for the Frank modulus and the index η:

$$K_A(T) = \frac{2T}{3a_0^2 n_0(T)}, \quad \eta(T) = \frac{27a_0^2 n_0(T)}{\pi}. \tag{40}$$

We see from (40) that as we approach the melting line [$n_0(T) \to 0$] we have $K_A(T) \to \infty$ and $\eta(T) \to 0$. This result corresponds to the existence of an orientational long-range order in the two-dimensional crystal. The condition for the (hexatic phase)–(ordinary liquid) transition, i.e., condition (39), and the expression for the index η do not depend on the

details of the interaction of the specific system (but they do depend on the lattice symmetry). The appearance of a free dislocation generates a displacement field $u \propto \ln R$, which disrupts the translational quasi-long-range order. The rotation angle which arises, however, satisfies $\omega \propto 1/R$, so the orientational quasi-long-range order persists until the density of free dislocations reaches the critical value [see (39)].

3. Disclination melting. A crystal can melt not only through the two transitions described above but also through a single transition, in the course of which disclination complexes dissociate, and free disclinations appear in the system. Because of the screening, the interaction between disclinations becomes a short-range interaction. When there is a disclination, the displacement field at large distances is of the form $u \propto R \ln R$, so the phase into which the crystal converts is completely disordered. Assuming that there are no dislocations in the liquid phase, we find an equation for the screening radius ξ from (25), (28), and (29) under the condition $r_0 m_0^{1/4} \ll 1$:

$$\Phi(x) = x^{\vartheta} - z \exp(-Q/x^2) = 0, \tag{41}$$

where

$$\vartheta = 4 + \frac{\pi K a_0^2 t^2}{144T} - \frac{\pi\alpha}{9T}, \quad Q = \frac{\pi^2 K a_0^2 t^2}{576T}, \tag{z}$$

$$z = \frac{\pi^2 K a_0^2 t^4}{8\cdot 3^{5/2} T} \exp\left(-\frac{E_c}{T}\right) \exp\left\{\frac{\pi\alpha(1+C)}{9T} - \frac{\pi K a_0^2 t^2 (1-C)}{144T}\right\}, \tag{a}$$

C is Euler's constant, $x = r_0/\xi$, $t = r_0/a_0$

$$\xi = \frac{1}{2}(c_0 m_0)^{-1/4} = \frac{1}{2}\left(\frac{\pi^2 \beta K m_0}{9}\right)^{-1/4}. \tag{c}$$

Equation (41) always has the solution $x = 0$, which corresponds to a crystalline phase. It is easy to see that a nontrivial solution arises under the condition

$$\Phi'(x) = 0. \tag{42}$$

From (41) and (42) we find

$$x^2 = 2Q/\vartheta. \tag{43}$$

Disclination melting thus occurs as a first-order transition, and a real solution exists under the condition $\vartheta > 0$. This condition holds if

$$T > \frac{1}{4}\left(\frac{\pi\alpha}{9} - \frac{\pi K a_0^2 t^2}{144}\right). \tag{44}$$

Comparing (44) with (34), we find that under the condition

$$\alpha > \alpha_c = K a_0^2 \left(\frac{9}{4\pi^2} + \frac{t^2}{16}\right) \tag{d}$$

dislocation pairs undergo dissociation before disclination complexes decay. In other words, under the condition $\alpha > \alpha_c$ the two-dimensional lattice melts through two continuous transitions. Qualitatively the same conclusion was reached by Alder and Wainwright,[27] who used the Monte Carlo method to find a lattice version of model (3). Unfortunately, the units of measure used in Ref. 27 prevent us from comparing the critical value of α calculated there with the value found for α_c in the present study. Alder and Wainwright[27] believe that a melting occurs as a first-order transition under the condition $\alpha < \alpha_c$. Their approach, however, did not consider the energy of a disclination core, E_c, or the relative size of the core, t, which appear in the coefficients of Eq. (41). It turns out that the behavior of the system depends strongly on these quantities.

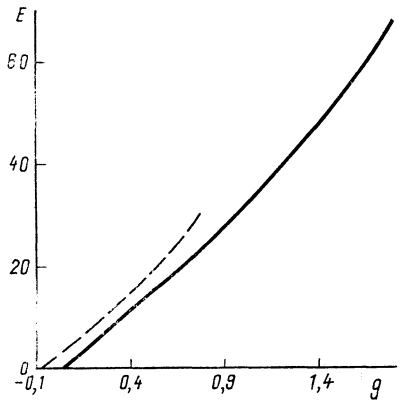

FIG. 1. $E = 16\pi E_c^*/Ka_0^2$ versus $g = \alpha/Ka^2$. Solid line—$t = 5$; dashed line—$t = 3$.

Substituting (43) into (41), we find an equation for the transition temperature:

$$\exp\left(-\frac{E_c}{T}\right) = \left(\frac{2Q}{\vartheta}\right)^{\vartheta/2} e^{\vartheta/2} \frac{8\cdot 3^{5/2}}{\pi^2 \beta K a_0^2 t^4} \exp\left\{-\frac{\pi\alpha(1+C)}{9T} - \frac{\pi K a_0^2 t^2 (1-C)}{144T}\right\}. \tag{45}$$

It can be seen from (45) that the transition temperature increases with increasing E_c and becomes higher than the temperature of the dislocation transition (34) at a certain E_c^*. Under the condition $E_c < E_c^*$, the melting thus occurs as a first-order transition, while under the condition $E_c > E_c^*$ it occurs as two continuous transitions. Substituting (34) into (45), we find an equation for E_c^*. Figure 1 shows $E = 16\pi E_c^*/Ka_0^2$ as a function of $g = \alpha/Ka_0^2$ for various values of t.

That the energy of the core of a defect is important in determining the type of transition has been pointed out in many papers (e.g., Refs. 7 and 18) on simulation of two-dimensional melting. Unfortunately, an unambiguous value of the energy of a defect core was not found there for a realistic model of the interacting particles. Various lattice representations of an elastic Hamiltonian [Hamiltonian (3) with $\alpha = 0$] are ordinarily used for the simulation.[7] Setting $t = 3$ in (45) (this is a fairly realistic value for the size of a defect core[29]), and setting $\alpha = 0$, we find $E \simeq 2.24$. Taking the energy of a dislocation core to be $\simeq 2E$, we find a fair agreement with estimates found by simulation.[7,18]

It can be seen from Fig. 1 that there are values of α^* at which E_c^* vanishes. At $\alpha < \alpha^*$ we should probably expect that the melting would always occur through two continuous transitions (the quantity α^* is independent of t).

Figure 2 shows E as a function of the relative size of the defect core for various values of α. Here there are also values of t^* at which we have $E_c^* = 0$, while at $t > t^*$ we would expect a two-step melting. Unfortunately, we know of no numerical simulations or actual experiments which have

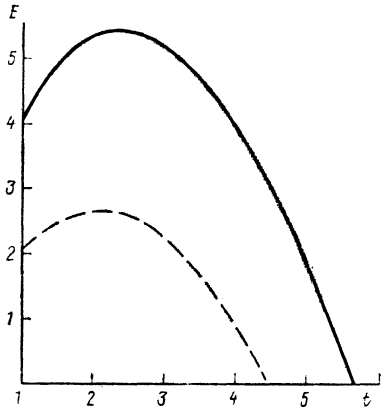

FIG. 2. $E = 16\pi E_c^*/Ka_0^2$ versus t. Solid line—$g = \alpha/Ka_0^2 = 0.1$; dashed line—$g = 0$.

been carried out on how melting is affected by the size of a defect core.

CONCLUSION

Many questions remain open and require further research. The simplified picture of dislocations and disclinations drawn by Hamiltonian (3) must be linked up with defects in real systems. Serious difficulties arise in attempts to determine the energy and size of a defect core. The behavior of the system near the point at which the first-order transition gives way to two continuous transitions remains unclear. It would be interesting to see a test of universal relation (39) for real systems.

The model which we have been discussing here is a significant simplification of real systems. Nevertheless, we believe that it is capable of describing a large number of transitions which are observed in the course of two-dimensional melting.

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