

Dislocation mechanism of crystal melting

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A field model is constructed for the description of a system of interacting dislocation lines. In this model the liquid–crystal transition corresponds to the appearance of infinitely long (unclosed) dislocation lines. It is shown that this transition is of first order.

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INTRODUCTION

It is known that a remarkable analogy exists between the magnetostatics of interacting currents and dislocation theory (see, e.g., Ref. 1). This allows us to propose an analogy between the mechanisms of the superconducting transition,¹ transitions in smectic-*A* liquid crystals,² and the transition in the theory of scalar electrodynamics,³ on the one hand, and the mechanism of dislocation-induced melting, on the other. In the first group of theories allowance for the long-wave fluctuations of the vector potential for a superconductor, the fluctuations of the director in a smectic-*A* liquid, or the gauge field in scalar electrodynamics leads to the conclusion that these are first-order transitions. We shall show in the present paper that allowance for dislocation interaction via the crystal deformation also lead to a first-order transition.

Attempts to involve dislocations in the description of crystal melting were made by various workers (see Halperin's review⁴ as well as the detailed description in Ref. 5), but they inevitably introduced simplifying assumptions concerning the form of the interaction of the dislocations and concerning their configuration statistics. (The most consistent with respect to allowance for the configuration statistics is the paper by Edwards and Warner,⁵ but it is not free of simplifications when account is taken of the dislocation interactions.)

Kleinert described in a recent preprint⁶ a formalism that makes possible a correct account of dislocation interaction. Unfortunately, apparently because the calculations are more unwieldy than ours, the calculated end result of his paper, corresponding to our Eq. (17), is accurate only to a numerical factor, i.e., it is of the same form as the result of the simple estimates.⁵

To describe a system of noninteracting dislocation lines we introduce three complex fields $\varphi_l(\mathbf{x}_i)$ ($l = 1, 2, 3$) (\mathbf{x}_i are the coordinates of the cubic-lattice points). We express the partition function in the form

$$Z = \int \prod_{\mathbf{x}_i} D\varphi_l(\mathbf{x}_i) D\varphi_l^*(\mathbf{x}_i) \left(1 + \sum_l \varphi_l(\mathbf{x}_i) \varphi_l^*(\mathbf{x}_i) \right) \times \exp \left\{ -\frac{1}{2} \sum_{(i,k)} J_{ik}^{-1} \varphi_l(\mathbf{x}_i) \varphi_l^*(\mathbf{x}_k) \right\}; \quad (1)$$

$J_{ik}^{-1} = 1/J$ for two nearest-neighbor sites and $J_{ik}^{-1} = 0$ in all other cases. This partition function is equal to the sum over all possible configurations of filaments of three types passing through the lattice points \mathbf{x}_i , and only one filament

can pass through one point. Each filament is marked by an arrow that indicates the current direction. Each segment of a filament of any sort enters with a weight J (we consider for simplicity the case of cubic symmetry, when all the filaments enter with equal weights). Each filament configuration enters thus the partition function with weight J^L , where L is the total length of the filaments of all sorts. The three different sorts of lines correspond to three different directions, along which the Burgers vectors of the dislocation can be directed. The partition function can be represented in the form

$$Z = \int D\varphi_l D\varphi_l^* \exp[-H\{\varphi_l, \varphi_l^*\}], \quad (2)$$

where

$$H\{\varphi_l, \varphi_l^*\} = \frac{1}{2} \sum_{(i,k)} J_{ik}^{-1} \varphi_l(\mathbf{x}_i) \varphi_l^*(\mathbf{x}_k) - \sum_i \ln \left(1 + \sum_l \varphi_l(\mathbf{x}_i) \varphi_l^*(\mathbf{x}_i) \right),$$

or, expanding the logarithm and changing to continual variables:

$$Z = \int D\varphi_l D\varphi_l^* \exp[-H\{\varphi_l, \varphi_l^*\}]; \quad (3)$$

$$H\{\varphi_l, \varphi_l^*\} = \frac{1}{2} \int d^2x \left\{ c |\nabla \varphi_l|^2 + \tau |\varphi_l|^2 + \left(\sum_l |\varphi_l|^2 \right)^2 \right\},$$

where

$$\tau = \sum_k J_{ik}^{-1} - 1, \quad c = \frac{1}{6} \sum_k J_{ik}^{-1} (\mathbf{x}_i - \mathbf{x}_k)^2.$$

The partition function (1) can also be written in the form

$$Z = \sum_{L,N} J^L n^N C(L, N), \quad (4)$$

where $C(L, N)$ is the number of different configurations on a lattice of N closed filaments with total length L . In our problem each filament enters with a factor $n = 6$, since there are only filaments of three sorts, in each of which the current can flow in two directions. From (4) we obtain for the average density of the dislocation line and for the average density of the dislocation loops:

$$c_m = \frac{\langle L \rangle}{V} = \frac{1}{V} J \frac{\partial \ln Z}{\partial J}, \quad (5)$$

$$c_c = \frac{\langle N \rangle}{V} = \frac{1}{V} n \frac{\partial \ln Z}{\partial n} \Big|_{n=6};$$

concrete expressions for c_m and c_c can be obtained from (2)

and (5) in the small-fluctuation approximation (see Ref. 7); at $\tau > 0$

$$c_m = \frac{n}{2} \int \frac{d^3k}{(2\pi)^3} \left(\frac{1}{J(\mathbf{k})} - 1 \right)^{-1},$$

$$c_c = \frac{n}{2} \int \frac{d^3k}{(2\pi)^3} \ln \left(\frac{1}{1-J(\mathbf{k})} \right). \quad (6)$$

We have presented here for c_m and c_c expressions obtained in first order in the fluctuations of the fields φ_l . We note that the main contribution to the integrals is made by integration with respect to momenta of the order of the reciprocal unit length of the lattice. This means that the main contribution to c_c and c_m is made by dislocation loops of size of the order of that of the lattice unit cell. Generally speaking, when account is taken of the interaction of the dislocations, the spectrum of the oscillations of the field φ is renormalized, but only at small momenta of the order of the reciprocal dislocation-interaction screening length (see below). Equations (6) are valid therefore also when account is taken of the dislocation interactions. An expression for the density of dislocations of finite length at $\tau < 0$ will be given later. The quantity J in the model Hamiltonian (2) is connected in simple fashion with the energy of the dislocation core per unit length:

$$J = e^{-E/\tau}. \quad (7)$$

A transition with formation of a line of infinite length takes place at a temperature t of the order E (in the self-consistent-field theory, at $zJ - 1 = 0$, where z is the lattice coordination number). The partition function (1) describes a system of nonintersecting dislocation lines. Replacing

$$\prod_i \left(1 + \sum_i \varphi_i(\mathbf{x}_i) \varphi_i^*(\mathbf{x}_i) \right)$$

in (1) by

$$\prod_i \left(1 + \sum_i \varphi_i \varphi_i^* + a \sum_i |\varphi_i|^4 + b \sum_{i,i'} |\varphi_i|^2 |\varphi_{i'}|^2 + c \sum_i |\varphi_i|^6 + \dots \right)$$

(with corresponding coefficients a , b , and c) we can obtain a similar description of a system with intersecting dislocation lines and with dislocation lines whose Burgers vectors are not simply equal to one of the unit vectors of the lattice but are arbitrary combinations of them. In such cases the problem still reduces to a partition function of the form (3) (the only possible difference is that owing to the cubic symmetry of the lattice the Hamiltonian $H\{\varphi_l \varphi_l^*\}$ in (3) can contain a term of the form $\sum_i \varphi_i^4$. We shall not consider hereafter this possibility, i.e., we confine ourselves to the isotropic case. This enables us to use only two constants in the description of the lattice properties and to simplify many expressions.

We recall that the partition function (1) describes a system of dislocations that do not interact via the lattice deformation. To describe the interaction we use the analogy between dislocation theory and magnetostatics. Thus, for example, the force acting on a dislocation is equal to⁸

$$d\mathbf{F} = [d\mathbf{l} \times (\sigma \mathbf{b})],$$

here $d\mathbf{l}$ is the length element of a dislocation with a Burgers vector \mathbf{b} and σ is the stress tensor. Comparing this expression

with the analogous one for the force $d\mathbf{F} = d\mathbf{l} \times \mathbf{H}$ acting on a current element, we see that for the three different orientations \mathbf{b}_l ($l = 1, 2, 3$) of the Burgers vector along the crystal axes we can introduce three different magnetic vectors \mathbf{H}_l , such that $\mathbf{H}_l = (\sigma \mathbf{b}_l)$ and the force acting on dislocation with a Burgers vector \mathbf{b}_l is simply $d\mathbf{F}_l = d\mathbf{l} \times \mathbf{H}_l$. The condition for the equilibrium of a deformed body takes in elasticity theory the form $\nabla^m \sigma_{ml} = 0$ or $\nabla \mathbf{H}_l = 0$, i.e., \mathbf{H}_l can be represented as the curl of a vector potential \mathbf{A}_l : $\mathbf{H}_l = \nabla \times \mathbf{A}_l$. Thus, the interaction of the dislocations with the medium can be taken into account by introducing for each field φ_l its own gauge vector potential¹⁾ \mathbf{A}_l :

$$H = \sum_l H_l = \frac{1}{2} \sum_l \int d^3x (c |(\nabla - i\mathbf{A}_l)\varphi_l|^2 + \tau |\varphi_l|^2 + \dots). \quad (8)$$

The Hamiltonian (8) is invariant to the gauge transformations

$$\mathbf{A}_l \rightarrow \mathbf{A}_l + \nabla \Theta_l, \quad \varphi_l \rightarrow \varphi_l e^{i\Theta_l},$$

where Θ_l are arbitrary functions.

Each of the Hamiltonian H_l describes the interactions between a system of conserved currents, having a Burgers vector \mathbf{b}_l , and the lattice deformation. It remains now only to express the lattice-deformation energy in terms of the same quantities \mathbf{A}_l .

The deformation energy of an isotropic body can be written in the form

$$E_{def} = \frac{1}{4\mu} \sigma_{lm}^2 + \frac{1}{4\mu} P \sigma_{ll}^2; \quad P = -\frac{\nu}{1+\nu}. \quad (9)$$

Here μ is the shear modulus and ν is the Poisson coefficient. It is simplest to substitute in (9) $\sigma_{lk} = \varepsilon^{kmr} \nabla^r A_l^m$.

In this case, however, it must also be noted that the condition that the tensor σ_{ik} be symmetric imposes stringent restrictions on the fields A_l^m . To take these restrictions into account, we introduce in the Hamiltonian an additional term of the form

$$\frac{1}{16\lambda} (\varepsilon^{iml} \nabla^m A_k^l - \varepsilon^{kml} \nabla^m A_i^l)^2.$$

We shall put $\lambda \rightarrow 0$ in the final expressions. Account will thus be taken only of field configurations A_k^l for which the stress tensor is symmetric. We write down now the total Hamiltonian of a system of interacting dislocations:

$$H = \frac{1}{2} \int d^3x \sum_l (c |(\nabla - i\mathbf{A}_l)\varphi_l|^2 + \tau |\varphi_l|^2) + g \left(\sum_l |\varphi_l|^2 \right)^2$$

$$+ \frac{1}{8\mu} (\varepsilon^{iml} \nabla A_k^l + \varepsilon^{kml} \nabla^m A_i^l)^2 + \frac{P}{8\mu} (\varepsilon^{iml} \nabla^m A_i^l)^2$$

$$+ \frac{1}{8\lambda} (\varepsilon^{iml} \nabla^m A_k^l - \varepsilon^{kml} \nabla^m A_i^l)^2. \quad (10)$$

To integrate over the fields A_l^m we must fix a gauge condition, which we write in the form $\nabla^m A_l^m = 0$. We shall need later the correlation functions of the fields A_l^m . To this end we express the terms of (10) that are quadratic in A in the form

$$\chi_{ll'}^{-imm'} A_l^m A_{l'}^{m'}, \quad (11)$$

where the matrix $\chi_{ll'}^{-imm'}$ takes in the momentum represen-

tation the form

$$\chi^{-1}(\mathbf{k})_{ii'}^{mm'} = \sum_{i',t'} k^i k^{t'} \left\{ \left(\frac{1}{8\mu} + \frac{1}{8\lambda} \right) \delta_{ii'} (\delta_{mm'} \delta_{it'} - \delta_{m't'} \delta_{m'i'}) \right. \\ \left. + \left(\frac{1}{8\mu} - \frac{1}{8\lambda} \right) \varepsilon^{i'm't'} \varepsilon^{l'm'r'} + \frac{P}{4\mu} \varepsilon^{i'm't'} \varepsilon^{l'm'r'} \right\} + \langle \varphi_l \rangle^2 \delta_{ii'} \delta_{mm'}$$

Here $\langle \varphi_l \rangle = \langle \varphi \rangle$ is the mean value of the fields φ_l ; we shall show below that $\langle \varphi_l \rangle^2$ is proportional to the average density of segments of infinite dislocation lines. We assume that all the $\langle \varphi_l \rangle$ are equal, i.e., that the high-temperature phase is isotropic. We find a matrix $\chi(\mathbf{k})_{ii'}^{mm'}$ such that when account is taken of the gauge condition $\nabla^m A^m = 0$ and of the current-conservation condition $\nabla^m j_l^m = 0$ the following equation holds:

$$A_i^m(\mathbf{k}) \chi^{-1}(\mathbf{k})_{ii'}^{mm'} \chi(\mathbf{k})_{i'i''}^{m'm''} j_{i''}^{m''}(\mathbf{k}) = A_i^m(\mathbf{k}) j_{i'}^{m'}(\mathbf{k}) \delta_{mm'} \delta_{ii'}$$

We consider first the case $\langle \varphi \rangle = 0$. After straightforward but cumbersome calculations we obtain

$$\chi_{m'm''}^{i'i''}(\mathbf{k}) = 8 \sum_{r,r',t,t'} \frac{k^r k^{r'} k^t k^{t'}}{k^8} \\ \times \left\{ \frac{\mu}{2} \delta_{i'i''} \delta_{ii'} (\delta_{m'm''} \delta_{rr'} - \delta_{m'r'} \delta_{m''r'}) \right. \\ \left. + \left(\frac{\lambda - \mu}{4} - \frac{\mu}{2} \frac{\lambda - \mu}{\lambda + \mu} \right) (\delta_{i''m''} \delta_{ii'} - \delta_{i''m''} \delta_{m'i'}) \right. \\ \left. \times (\delta_{i'm'} \delta_{rr'} - \delta_{i'r} \delta_{m'r}) \right. \\ \left. + \frac{\mu}{2} \frac{\lambda - \mu}{\lambda + \mu} \delta_{ii'} (\delta_{i'r} \delta_{i''m''} \delta_{m'r'} - \delta_{i''m''} \delta_{i'r} \delta_{m'r'}) \right. \\ \left. - \delta_{i'r} \delta_{i''m''} \delta_{m'r'} + \delta_{i'm'} \delta_{i''m''} \delta_{rr'} \right. \\ \left. - \frac{P}{2\mu + 4P/\mu} \varepsilon^{i'm'r'} \varepsilon^{i''m''r} \delta_{ii'} \right\}. \quad (12)$$

This expression becomes simpler in the limit as $\lambda \rightarrow 0$. We note that $\chi_{ii'}^{mm'} j_l^m j_l^{m'}$ is the interaction energy of the dislocation currents. This energy is not uniquely defined,¹ accurate to terms whose integral along a closed dislocation line is zero. In our notation these are the terms of (12) which contain factors of the form $k^r \delta_{rm'}$ or $k^r \delta_{rm''}$. Accurate to such terms, Eq. (12) coincides in the limit as $\lambda \rightarrow 0$ with the expression obtained by Peach and Koehler⁸ for the dislocation-interaction energy,

$$E = \iint M_{ii'}^{mm'}(\mathbf{r}_1 - \mathbf{r}_2) j_l^m(\mathbf{r}_1) j_l^{m'}(\mathbf{r}_2) d\mathbf{r}_1 d\mathbf{r}_2,$$

where

$$M_{ii'}^{mm'}(\mathbf{k}) = 2\mu \sum \frac{k^r k^{r'}}{k^4} \left[\delta_{mm'} (\delta_{ii'} \delta_{rr'} - \delta_{i'r} \delta_{i''r'}) \right. \\ \left. + \varepsilon^{i'm'r} \varepsilon^{i''m'r'} + \frac{2\nu}{1-\nu} \varepsilon^{i'm'r} \varepsilon^{i''m'r'} \right] \quad (13)$$

(in our notation).

We consider now the case $\langle \varphi \rangle \neq 0$. It can be easily seen that it suffices in this case to replace in (12) μ , λ , and P by $\mu^*(\mathbf{k})$, $\lambda^*(\mathbf{k})$ and $P^*(\mathbf{k})$, so that

$$1/\mu^*(\mathbf{k}) = 1/\mu + \langle \varphi \rangle^2 / k^2, \quad 1/\lambda^*(\mathbf{k}) = 1/\lambda + \langle \varphi \rangle^2 / k^2, \\ P^*(\mathbf{k}) / \mu^*(\mathbf{k}) = P / \mu. \quad (14)$$

The unclosed dislocation currents leads thus to screening of

the interaction (the effective elasticity μ^* vanishes over scales of the order of $r_c = (\mu^{1/2} \langle \varphi \rangle)^{-1}$).

In the limit as $\lambda \rightarrow 0$ we obtain ultimately

$$\chi_{i'i''}^{m'm''}(\mathbf{k}) = 8 \sum \frac{k^r k^{r'} k^t k^{t'}}{k^4 (k^2 + \mu \langle \varphi \rangle^2)} \\ \times \left\{ \frac{\mu}{2} \delta_{i'i''} \delta_{ii'} (\delta_{m'm''} \delta_{rr'} - \delta_{m'r'} \delta_{m''r'}) \right. \\ \left. + \frac{\mu}{4} (\delta_{i''m''} \delta_{ii'} - \delta_{i''m''} \delta_{m'i'}) (\delta_{i'm'} \delta_{rr'} - \delta_{i'r} \delta_{m'r}) \right. \\ \left. - \frac{\mu}{2} \delta_{ii'} (\delta_{i'r} \delta_{i''m''} \delta_{m'r'} \right. \\ \left. - \delta_{i''m''} \delta_{i'r} \delta_{m'r'} - \delta_{i'r} \delta_{i''m''} \delta_{m'r'} + \delta_{i'm'} \delta_{i''m''} \delta_{rr'}) \right. \\ \left. - \frac{\mu}{2} \frac{Pk^2}{(1+2P)k^2 + \mu \langle \varphi \rangle^2} \varepsilon^{i'm'r'} \varepsilon^{i''m''r} \delta_{ii'} \right\}. \quad (15)$$

Let us estimate, using the expression for the correlation function of the fields, the fluctuation contribution from these fields. It follows from (10) that

$$dH\{\langle \varphi \rangle\} / d\langle \varphi \rangle = 6\tau \langle \varphi \rangle + 36g \langle \varphi \rangle^3 + 2\langle A_l^2 \rangle \langle \varphi \rangle, \quad (16)$$

with

$$\langle A_l^2 \rangle = \int \frac{d^3 k}{(2\pi)^3} \chi_{ii'}^{mm}(\mathbf{k}) = \text{const} - 3U \langle \varphi \rangle, \quad (17)$$

where

$$U = \frac{\mu^{3/2}}{\pi} \left[1 - \frac{2P}{3(1+P)^{3/2}} - \frac{2P}{3(1+P)^{3/2}} - \frac{2}{3} (1 - (1+P)^{1/2}) \right].$$

Thus, allowance for the long-wave fluctuations of the fields leads to a term of the form $\langle \varphi \rangle^3$ in $H\{\langle \varphi \rangle\}$. The transition from $\langle \varphi \rangle = 0$ to $\langle \varphi \rangle \neq 0$ proceeds jumpwise, with formation of a finite density of unclosed dislocation lines.

From (5), (16), and (17) we obtain for the density of the segments of unclosed distribution lines:

$$c_m^\infty = \langle \varphi \rangle^2 = \begin{cases} (U/9g)^2 & \text{at transition point } \tau^* = U^2/27g, \\ \left(\frac{U + (U^2 - 24g\tau)^{1/2}}{12g} \right)^2 & \text{at } \tau < \tau^*. \end{cases} \quad (18)$$

We have confined ourselves here to the self-consistent-field approximation. The reason is that, unlike in Eqs. (6), which are not greatly altered by allowance for the dislocation interactions, at $\tau < \tau^*$ the system is in a new state, the transition into which is due just to the dislocation interaction. The oscillation spectrum now depends substantially on the interaction constant μ . The corresponding calculations for the quantities c_c and c_m can be performed in first order in the fluctuations, but they are not meaningful because the phase with $\langle \varphi \rangle \neq 0$ is a liquid.

We recall that in our problem the relation between the real physical temperature T and the "model temperature" J is such that small J and $\langle \varphi \rangle \neq 0$ correspond to the high-temperature phase of a physical system, and large J and $\langle \varphi \rangle = 0$ to the low-temperature phase. Since the theory is gauge-invariant at $\langle \varphi \rangle \neq 0$, no unphysical Goldstone oscillations arise—transverse phonons in the low-temperature phase are outside the scope of our model. The point is that we represent each i -th column of the stress tensor in the form of a curl

of a vector field. Generally speaking this column, being an arbitrary vector, can be represented as the sum of a curl and a gradient

$$V_i^k = \nabla_i \Phi^k + \epsilon_{ijl} \nabla_j A_l^k.$$

Allowance for the phonons in our theory would correspond to introduction of potentials Φ^k and to a corresponding averaging over them. This would lead to a certain renormalization of the parameters of the Hamiltonian (10).

From (16) and (17) we obtain the latent heat of melting at the transition point

$$L = T \left\{ \frac{\partial H \langle \langle \varphi \rangle \rangle}{\partial \tau} - \frac{\partial H \langle \langle \varphi \rangle = 0 \rangle}{\partial \tau} \right\} \frac{\partial \tau}{\partial T} = \frac{E}{T} \left(\frac{U}{g} \right)^2. \quad (19)$$

The region of validity of the obtained relations can be found from the condition that the value of τ^* at which the transition takes place is within the region of validity of the self-consistent-field theory:

$$U^2/g > g^2/c^3 \quad (20)$$

for for the problem in the lattice formulation: $g \sim 1$ and $c^3 = 1$. The condition (20) is simply the condition that the shear modulus μ be large. Since we used the dimensionless quantity $\mu = \mu^*/T$ and $T \sim E$, we obtain

$$\mu^* > E.$$

In the opposite case, when self-consistent-field estimates show that the transition takes place in the region of the strong fluctuations, the situation is unclear. A similar question of the form of the transition in the strong-fluctuation

region in a simpler model with one complex field φ and with one gauge field A , which describes type-II superconductors, has remained open for a long time. Recently Dasgupta and Halperin¹⁰ have shown that this is a second-order transition. Allowance for the fluctuations in our model can therefore change the order of the transition from first to second.

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¹⁰A detailed substantiation of the introduction of a vector potential to describe the interaction between currents is contained in Appendix 2 of Ref. 9.

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