Disclinations as Origin of First-Order Transitions in Melting.

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Summary. – We demonstrate that within our gauge theory of defects and stresses in three dimensions, disclinations play a crucial role in making the melting transition of first order.

It is well known that any model of defect melting must account for the proliferation of disclinations. Otherwise, it is impossible to transform a crystal into a proper liquid without directional memory. In two dimensions [1], the standard treatment proceeds in two steps: first, one considers a pure dislocation model and applies the methods of Kosterlitz-Thouless to find the dislocation pair unbinding temperature; then one argues that in this phase, which has somewhat exotic properties, the disclinations should form a Coulomb-like gas which can once more undergo a pair transition [1].

Unfortunately, such a procedure ignores the feedback of disclinations upon the process of dislocation melting. It is the purpose of this note to show that this feedback is essential in making the transition first order. For physical reasons, we shall study only three-dimensional systems [*].

Our result resolves the outstanding puzzle as to the difference between the melting transition and the superfluid-normal transition in ^{4}He. That system contains only vortex lines which are analogous to dislocations, and there are no disclinations. The proliferation of vortex or dislocation lines alone « normally » leads to a second-order phase transition [2].

Let us specify what we mean by « normally ». Crystals as well as superfluid ^{4}He are nonlinear systems. Their long–wave-length excitations are free phonons with very

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[1] B. I. HALPERIN and D. R. NELSON: *Phys. Rev. Lett.*, **41**, 121 (1978); *Phys. Rev. B*, **19**, 2457 (1979).
[*] The two dimensional case is treated in H. KLEINERT: *Phys. Lett. A*, **95**, 381 (1983).
[2] H. KLEINERT: *Phys. Lett. A*, **93**, 86 (1982).

simple-bending energies

(1) $$f_{\text{crystal}} = \frac{\mu}{2} (\partial_i u_j)^2 + \frac{1}{2} (\lambda + \mu)(\partial_i u_i)^2 \,, \qquad f_{\text{4He}} = \frac{\varkappa}{2} (\partial_i \varphi)^2 \,,$$

where u_i are atomic displacements, φ is an angle between zero and 2π and μ, λ and $\varkappa$ are elastic constants. The nonlinearities at short distances give rise to defects. These can be included in an idealized way by writing the energies (1) in terms of lattice gradients $\nabla_i u_j(x) = u_j(x + i) - u_j(x)$ and allowing for jumps by multiples of the lattice spacing [3]. Similarly, the gradient $\nabla_i \varphi$ can jump by multiples of 2π [2]. If such jumps take place over some surface, its boundary becomes an idealized dislocation or a vortex line [4]. The surface itself is physically irrelevant [5].

Such an idealized line has a self-energy which is entirely due to linear elasticity. It is given by the lattice Coulomb potential at the origin $v(0) = - (1/\nabla_i \nabla_i)(0) \approx 0.253$. This acts as a « core energy » suppressing the thermal creation of lines. It can be shown that lines with this core energy undergo a second-order phase transition [6]. This is what we mean by « normally ».

Field-theoretically, the situation is as follows: The system of random lines and their elastic interactions can be described by a disorder gauge theory which has the same form as the Ginzburg-Landau theory of superconductivity, if the order parameter ψ and magnetic potential A are interpreted as disorder and stress, respectively [2-4]. This theory is characterized by a specific value of K which is the ratio of the two length scales of this system (magnetic penetration/coherence length). The condition $K \gtrless 1/\sqrt{2}$ separates type-II from type-I superconductivity. The core energy reflects itself in the strength of the short-range steric repulsion between line elements. In the Ginzburg-Landau description, this is parametrized by the coupling constant g of the quartic $|\psi|^4$ term. The normal case described above amounts to $K = K_{\text{norm}} = 3\sqrt{3}/2\pi = 1.17/\sqrt{2}$ [2]. Thus it lies in the type-II regime where the transition is of second order [6].

How can it then be that dislocations undergo a first-order phase transition? A possible answer is suggested by an old argument by HALPERIN, LUBENSKY and MA [7], according to which the superconductive transition at low K should be first order. The value of K where this really takes place was estimated to be [6] $K \sim 0.8/\sqrt{2}$. This led us to conclude [4] that if the dislocation lines have a strongly suppressed steric repulsion, which amounts to a negative core energy in addition to the purely elastic one, the transition could become first order. Our conclusion was confirmed in two dimensions by an independent Monte Carlo calculation [8]. What remained unclear, however, was the origin of this reduction in core energy.

While such an explanation was certainly a theoretical possibility, we now believe that it misses an important physical aspect of the problem, namely the fact that crystals, unlike ^{4}He, support another type of linelike topological defects. These are the defects of rotational symmetry, the disclinations. We shall now demonstrate that these do, indeed, make melting a first-order transition without subtle manipulation of core energies.

[3] H. KLEINERT: *Phys. Lett. A*, **94**, 295 (1982); to be published in *Lett. Nuovo Cimento*.
[4] H. KLEINERT: *Lett. Nuovo Cimento*, **34**, 464, 471 (1983); *Phys. Lett. A*, **89**, 256 (1983).
[5] H. KLEINERT: *Lett. Nuovo Cimento*, **34**, 209 (1982).
[6] H. KLEINERT: *Lett. Nuovo Cimento*, **35**, 405 (1982).
[7] B. I. HALPERIN, T. C. LUBENSKY and S. K. MA: *Phys. Rev. Lett.*, **32**, 292 (1974).
[8] Y. SAITO: *Phys. Rev. Lett.*, **48**, 1114 (1982); *Phys. Rev. B* (in press).
[9] H. KLEINERT: *Phys. Lett. A*, **95** (1983).

The starting point is the lattice model of dislocation melting as developed in ref. [3]. Using reduced dimensionless variables for stress and defining $\tau = \pi^2 T/\mu a^3$, where T = temperature, μ = shear module, we can write the partition function of a crystal as

$$(2) \qquad Z = \prod_{x,i,j} \int \mathrm{d}\bar{h}_{ij}(x) \sum_{\bar{\eta}_{ij}(x)} \delta_{\overline{\nabla}_i \bar{\eta}_{ij}(x),0} \exp\left[-\tau \sum_{x,i,j} \left(\bar{\sigma}_{ij}^2 - \frac{\nu}{1+\nu}\bar{\sigma}_{ii}^2 \right) + 2\pi i \sum_{x,i,j} \bar{\eta}_{ii}\bar{h}_{ij} \right] ,$$

where $\nu = \frac{1}{2}\lambda/(\lambda + \mu)$ is the Poisson number and the symmetric tensor $\bar{h}_{ij}(x)$ is the gauge field of stress in terms of which

$$(3) \qquad \bar{\sigma}_{ij}(x) = \varepsilon_{ikl}\varepsilon_{jmn}\overline{\nabla}_k\overline{\nabla}_m \bar{h}_{ln}(x - l - n) .$$

The sum over symmetric integer tensors $\bar{\eta}_{ij}$ with $\overline{\nabla}_j\bar{\eta}_{ij} = 0$ accounts for the defects. These can split into dislocations and disclinations with densities $\bar{\alpha}_{ij}$, $\bar{\theta}_{ij}$, respectively, as

$$(4) \qquad \bar{\eta}_{ij} = \bar{\theta}_{ij} - \frac{1}{2}\overline{\nabla}_m\left(\varepsilon_{mjl}\bar{\alpha}_{li} + (i \leftrightarrow j) + \varepsilon_{ijl}\bar{\alpha}_{lm} \right) .$$

The densities satisfy the conservation laws $\overline{\nabla}_j\bar{\theta}_{ij} = 0$ and $\overline{\nabla}_j\bar{\alpha}_{ij} = \varepsilon_{ikj}\bar{\theta}_{kj}$. Thus disclinations form closed random lines. Dislocations, on the other hand, form closed lines only as long as there are no disclinations. These can act as sources or sinks. Let us neglect this latter possibility, since it can be shown to have no important effect upon the melting process [9]. Then the sum over $\bar{\alpha}_{ij}$ with $\overline{\nabla}_j\bar{\alpha}_{ij} = 0$ is a sum over three independent sets of closed nonbacktracking random loops. Its partition function can be summed by a disorder field theory [4,10] to which the gauge field is coupled, in the long–wave-length limit, via the covariant derivative [11]

$$(5) \qquad D_i\psi_j \approx (\partial_i - i\varepsilon_{jlk}\partial_j\bar{h}_{ki})\psi_l .$$

If there were no disclinations, this disorder field theory would have a second-order phase transition [2]: Above a certain temperature τ_c, each $|\psi_l|$ takes a nonzero expectation value and the transverse phonons lose their long-range propagation (Meissner effect).

In the long–wave-length limit, the correlation function of $\bar{h}_{ij}$ takes the form

$$(6) \qquad \langle \bar{h}(x)\bar{h}(0) \rangle \underset{|x|\to\infty}{\sim} \frac{1}{\tau}\sum_k \exp[ikx] \frac{1}{k^4 + |\psi|^2|k|^2} ,$$

where we have left out inessential indices [9], for simplicity. For large distances, this is proportional to a lattice Coulomb potential $v(x)$,

$$(7) \qquad \langle \bar{h}(x)\bar{h}(0) \rangle \underset{|x|\to\infty}{\sim} \frac{1}{\tau|\psi|^2} v(x) .$$

Let us now add disclinations. By neglecting inessential projection matrices [3,4], their partition function reads

$$(8) \qquad \exp\left[-\frac{4\pi^2}{\tau|\psi|^2} \right] \sum_{x,x'} \theta_{ij}(x)v(x - x')\theta_{ij}(x') .$$

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[10] H. KLEINERT: *Erice Lectures 1982*, edited by A. ZICHICHI (to be published).
[11] H. KLEINERT: *Lett. Nuovo Cimento*, **34**, 471 (1982).

Thus we see that in the presence of dislocations, *i.e.* when $|\psi| \neq 0$, disclinations form a system of random loops which have precisely the same long-range interactions as the dislocation loops had in the perfect crystal, with a force which becomes weaker as the dislocation density increases. Since $|\psi|^2$ accompanies τ, one may describe the increase of $|\psi|$ also as an increase of the effective temperature of the disclination system. In other words, if at a fixed physical temperature the system is filled with more and more dislocations, this is conceived by the disclinations just as a heating process. Thus at fixed τ, there exists a value $|\psi|_c$ above which the disclinations underg othe same type of phase transition as a function of $|\psi|$ as previously the dislocations as a function of τ. It is this property of the combined defect system which makes the phase transition of first order.
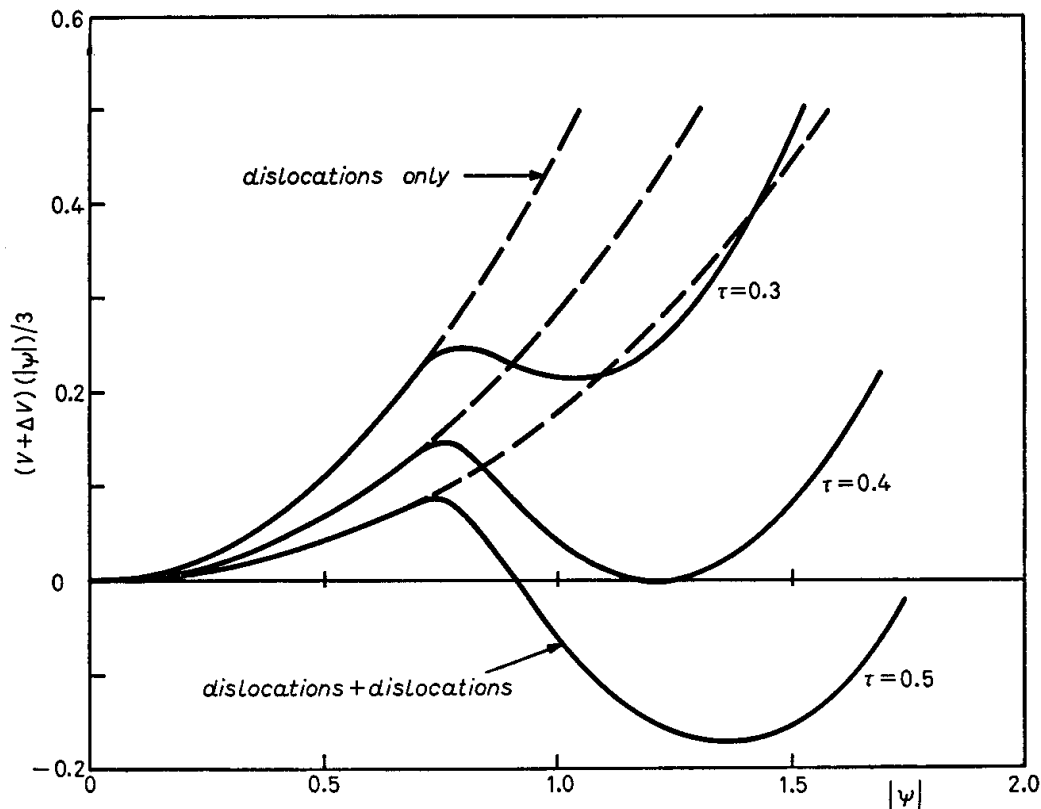

Fig. 1. – The depression in the effective potential of dislocations caused by disclination melting. This makes the transition first order. The explicit form of the potential is (*)

$$(V + \Delta V)(|\psi|) = \sum_i \left\{ \frac{1}{4} \left(\frac{0.83}{\tau} - 1 \right) |\psi|^2 + \frac{1}{64} |\psi|^4 - \Theta(|\psi|^2 - 2v(0)) \left(\frac{2v(0)}{|\psi|^2} - 1 \right)^2 \right\}.$$

In order to see this, consider in a Landau approximation the effective potential as a function of the dislocation field $|\psi|$ alone. Neglecting disclinations, this has a stable minimum at the origin for $\tau < \tau_c$ and would destabilize for $\tau > \tau_c$ (see fig. 1). Consider now the modification brought about by disclinations. As long as $|\psi|$ is smaller than $|\psi_c| = = \sqrt{2v(0)}$, the core energy of disclinations is so large that they cannot appear in the crystal. Thus the potential remains unchanged. Above $|\psi_c|$, however, the force between disclinations becomes so weak that these proliferate, thereby lowering the ef-

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(*)   The pure dislocation part of V is taken from (³), the disclination part is the minimum of an analogous disorder field potential form (⁸).

fective potential. The deviation begins quadratically in $(|\psi| - |\psi_c|)$ and becomes constant for large $|\psi|$ (see fig. 1). This leads to a depression in the defective potential. If the temperature is raised towards τ_c, there will be a value $\tau_{melt} < \tau_c$, where the minimum at the depression becomes equal in energy with the origin. There both, dislocations and disclinations, proliferate in a single first order phase transition. The transition entropy can be estimated as $\Delta S \sim 2.4$ per cell (in units of the Boltzmann constant).

A more detailed quantitative discussion will be presented elsewhere [12].

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[12] H. KLEINERT: *Gauge Theory of Defects and Stresses* (New York, N.Y., 1984).