DISCLINATIONS AND FIRST ORDER TRANSITIONS IN 2D MELTING

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Received 12 August 1982

We present a unified analysis of two-dimensional defect melting involving both dislocations and disclinations. This permits the study of the feedback between the two types of defects and explains the first order of the melting transition.

Recently, the first order of the melting transitions in three dimensions has been traced back to the existence of disclination lines [1]. These form a reservoir of entropy which, in the crystalline state, is frozen, but which opens up as soon as dislocations proliferate. This, in turn, favors the formation of further dislocations. It is this feedback which makes the transition first order. Previous discussions [2] investigate disclinations only in an exotic premolten (in triangular lattices called "hexatic") phase in which case they find a sequence of continuous Kosterlitz–Thouless transitions. There is a possibility of a first order transition within a pure dislocation model if these have a particularly small core energy. This was first noticed by the author in three dimensions on theoretical grounds [3] [‡1] and confirmed independently in two dimensions via Monte Carlo calculations [5]. What remained unclear, however, was the origin of the small core energy. In this note we shall point out that the original choice of core energy [2], which was made in order to allow for a carefree application of the dilute gas techniques of Kosterlitz–Thouless, was unphysical. It destroyed an important physical property of dislocations; namely the possibility of their stringing up along a line, with the Burgers vectors pointing transverse to it, thereby forming a disclination. In a two-dimensional crystal this is always possible. The resulting disclination is a point singularity at the end point of the string. The string has no physical reality whatsoever, in particular no energy. Just as the "Dirac string" of a magnetic monopole, it can be chosen to run along any direction in space. A core energy associated with the Burgers vectors [2] makes strings energetic and thus destroys the physics of the crystal. It is the purpose of this note to give a proper treatment of core energies. This automatically allows for disclinations and leads to a first order melting transition, just as in the three dimensional theory [1].

The elastic energy is

$$f = \mu u_{ij}^2 + \tfrac{1}{2}\lambda u_{ii}^2 = (1/4\mu)\{\sigma_{ij}^2 - [\nu/(1+\nu)]\,\sigma_{ii}^2\}\,,$$

where μ, λ are the Lamé constants, ν is the Poisson number $\{\nu = \lambda/[(D-1)\lambda + 2\mu]$ in D dimensions$\}$, and σ_{ij}, u_{ij} are stress and strain tensors, respectively. Since $\bar{\nabla}_i \sigma_{ij} = 0$ [‡2], one can write $\sigma_{ij}(x) = 2\pi T \epsilon_{ik}\epsilon_{jl}\nabla_k \nabla_l \phi(x)$ and the field $\phi(x)$ has the advantage of coupling locally to dislocations and disclinations via an interaction energy

$$\frac{E_{\text{int}}}{T} = 2\pi \sum_x b_i(x)\epsilon_{ij}\nabla_j\phi(x) + m(x)\phi(x)\,, \tag{1}$$

[1] Supported in part by the National Science Foundation, grant number PHY77-27084.

‡1 For further discussions, see ref. [4].

‡2 We work on a simple cubic lattice where x are the sites and i the positively oriented lines. Then $\nabla_i\phi(x) \equiv \phi(x+i) - \phi(x)$, $\bar{\nabla}_i\phi(x) \equiv \phi(x) - \phi(x-i)$.

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where $b_i(x), m(x)$ are the integer valued fields of Burgers vectors and Frank scalars, respectively.

Actually, the two defects are not independent of each other. For example, disclinations can be built from a string of dislocations. Thus we can find them in any proper pure dislocation model. In order to study their effect we find it convenient to display them explicitly in the partition function by writing on arbitrary field of Burgers vectors as

$$b_i(x) = \epsilon_{ij}\bar{\nabla}_j n(x) + \delta_{i,2} \sum_{x'_1=x_1} m(x'_1, x_2) .$$

The first term $b_i^{\mathrm{T}}(x) = \epsilon_{ij}\bar{\nabla}_j n(x)$ is an integer valued transverse vector field ($\bar{\nabla}_i b_i^{\mathrm{T}} = 0$). The smallest b_i^{T} configuration is a closed square, say $b_1(\mathbf{0}) = 1, b_2(\mathbf{1}) = 1, b_1(\mathbf{2}) = -1, b_2(\mathbf{0}) = -1$. This may be viewed as a Shockley point defect. With this separation, the partition function of the pure dislocation model can be reexpressed in the form

$$Z = \prod_x \int_{-\infty}^{\infty} \mathrm{d}\phi(x) \sum_{b_i^{\mathrm{T}}(x)} \sum_{m(x)} \left[\exp\left(-\frac{\pi t}{2} \sum_x (\nabla\bar{\nabla}\phi)^2 + 2\pi \mathrm{i} \sum_x (b_i^{\mathrm{T}} \epsilon_{ij} \bar{\nabla}_i \phi + m\phi)\right)\right] , \qquad (2)$$

where we have set

$$t \equiv 2\pi T/\mu(1+\nu) = \pi T(2\mu + \lambda)/(\mu + \lambda) .$$

We shall now demonstrate that the b_i^{T} configurations liberate disclinations and lead, in analogy with the three-dimensional case, to a first order melting transition via a similar backfeeding mechanism. Thus, unless artificial [‡3] model core energies suppress these configurations, also two-dimensional melting, will be of first order. Natural core energies which can arise from nonlinear elasticity would lead to a Boltzmann factor

$$\exp\left[-\frac{1}{t}\left(E^{\mathrm{T}} \sum_x b_i^{\mathrm{T}^2} + E' \sum_x m^2\right)\right] .$$

If the ϕ field is integrated out, it gives rise to a potential between m's which behaves for large r as

$$v_4(x) \equiv \sum_{\boldsymbol{k}} \exp(\mathrm{i}\boldsymbol{k}\boldsymbol{x})(K^2 + \delta^2)^{-2} \sim 1/4\pi^2\delta^2 + (1/8\pi) r^2 (\log r + c) + \ldots , \qquad (3)$$

where

$$K^2 \equiv \sum_i |K_i|^2 = \sum_i |\exp(\mathrm{i}k_i) - 1|^2 = 4 - 2(\cos k_1 + \cos k_2)$$

for a simple cubic lattice and $\delta \sim 0$ is a regulator mass. The potential between b_i^{T}'s is

$$v_{ij}^{\mathrm{T}}(x) \equiv \sum_{\boldsymbol{k}} \exp(\mathrm{i}\boldsymbol{k}\boldsymbol{x}) \frac{\delta_{ij}K^2 - K_i^* K_j}{(K^2 + \delta^2)^2} \approx -(1/4\pi)(\delta_{ij} \log r - x_i x_j / r^2) - (1/4\pi)(c + \tfrac{3}{2})\,\delta_{ij} + \ldots , \qquad (4)$$

but due to the restriction $\bar{\nabla}_i b_i^{\mathrm{T}} = 0$, the angular dependence is automatically enforced by the transversality condition and we can write the interaction as

$$-\frac{2\pi}{t} \sum_{x,x'} b_i^{\mathrm{T}}(x) v_{ij}^{\mathrm{T}}(x - x') b_j^{\mathrm{T}}(x') = -\frac{2\pi}{t} \sum_{x,x'} b_i^{\mathrm{T}}(x) v_2(x - x') b_i^{\mathrm{T}}(x') ,$$

‡3 Note that if core energies are a result of elasticity only, they are diagonal in $b_i^{\mathrm{T}^2}$, due to the transverse coupling to stress. The "derivation" of the core energy $\propto b_i^2$ in ref. [2] overlooks this.

where $v_2(x)$ is the Coulomb potential

$$v_2(x) = \sum_k \exp(\mathrm{i}kx) \frac{1}{K^2 + \delta^2} \underset{r\to\infty}{\sim} -\frac{1}{2\pi}(\log r + c + 1) . \tag{5}$$

The number c diverges like $-\log \delta$. The infinities give rise to a factor in Z

$$\exp\left\{ -\frac{2\pi}{t}\left[v_4(0)\left(\sum_x m\right)^2 + v_2(0)\left(\sum_x b_i^{\mathrm{T}}\right)^2 \right]\right\} , \tag{6}$$

which shows that only neutral systems of disclinations and transverse dislocations contribute. The remaining subtracted potentials $v_4'(x) \equiv v_4(x) - v_4(0), v_2'(x) \equiv v_2(x) - v_2(0)$ vanish at the origin such that the potential energies are

$$\frac{2\pi}{t}\left(\sum_{x\neq x'} m(x) v_4'(x-x') m(x') + \sum_{x\neq x'} b_i^{\mathrm{T}}(x) v_2'(x-x') b_i^{\mathrm{T}}(x') \right) . \tag{7}$$

In the dislocation part it will be convenient to also remove the next neighbor value

$$v_2'(1) = \sum_k [\exp(\mathrm{i}k_i) - 1]\, K^{-2} = \frac{1}{2}\sum \frac{\cos k_1 - 1}{4 - 2(\cos k_1 + \cos k_2)} = -\tfrac{1}{4} \tag{8}$$

since then we can write

$$\frac{2\pi}{t}\sum_{x\neq x'} b_i^{\mathrm{T}}(x) v_2'(x-x') b_i^{\mathrm{T}}(x') = \frac{2\pi}{t}\sum_{x\neq x'}'' b_i^{\mathrm{T}}(x) v_2''(x-x') b_i^{\mathrm{T}}(x') + \frac{\pi}{2t}\sum_x b_i^{\mathrm{T}}(x)^2 , \tag{9}$$

where the sum $\Sigma''_{x\neq x'}$ begins with second next neighbors and the potential $v_2''(x) = v_2'(x) - v_2'(1)$ is well approximated by $-(1/2\pi)[\log r + \log\sqrt{8}\exp(\gamma - \frac{1}{2}\pi)]$. Forgetting for a moment the subtractions in $v_4(x)$, we can now rewrite the partition function as

$$Z = \prod_x \int_{-\infty}^{\infty} \mathrm{d}\phi(x) \sum_{b_i^{\mathrm{T}}(x)} \sum_{m(x)} \exp\left[-\frac{\pi t}{2}\sum_x (\nabla^2\phi)^2 + 2\pi\mathrm{i}\sum_x (b_i^{\mathrm{T}}\epsilon_{ij}\nabla_j''\phi + m\phi) \right.$$

$$\left. -\frac{1}{t}\left((E^{\mathrm{T}} + \tfrac{1}{2}\pi)\sum_x b_i^{\mathrm{T}2} + E'\sum_x m^2 \right) \right] , \tag{10}$$

where ∇'' implies that $-\nabla''\bar{\nabla}''/(\nabla\bar{\nabla})^4 \equiv v_2''(x)$ i.e. in Fourier space

$$K''^2 \equiv (K^2 + \delta^2)\{1 - [v_2(0) + v_2'(1)]\,\delta_{k,0}(K^2 + \delta^2)\} .$$

This partition function can now be discussed in analogy with the three-dimensional case: Since b_i^{T} satisfies $\bar{\nabla}_i b_i^{\mathrm{T}} = 0$, the Burgers vectors line up to form a set of closed random walks. Their sum can be converted into a complex disorder field theory and, close to a critical point, Z takes the form [3,6] [‡4]

$$Z = \prod_x \int_{-\infty}^{\infty} \mathrm{d}\phi(x) \sum_{m(x)} \prod_{x,l} \int \mathrm{d}\psi_l(x)\, \mathrm{d}\psi_l^+(x) \exp\left\{ -\frac{\pi t}{2}(\nabla^2\phi)^2 + 2\pi\mathrm{i}\sum_x m\phi - \frac{1}{t}E'\sum_x m^2 \right.$$

$$\left. -\sum_{x,l}\left[\left(\frac{E^{\mathrm{T}} + \frac{1}{2}\pi}{\pi t} - \frac{1}{4} \right)|\psi_l|^2 + \frac{1}{4\pi}|(\nabla_i - \mathrm{i}2\pi\epsilon_{ij}\nabla_j''\phi)\psi_l|^2 + \tfrac{1}{64}|\psi_l|^4 + \mathrm{O}(|\psi|^6) \right] \right\} . \tag{11}$$

‡4 At the mean field level, the mass term would actually be $[(E^{\mathrm{T}} + 2)/\pi t - 1/4]\,|\psi_l|^2$. Knowing the actual place of the phase transition in the 2D Ising model, we have renormalized the number 2 to $\pi/2$.

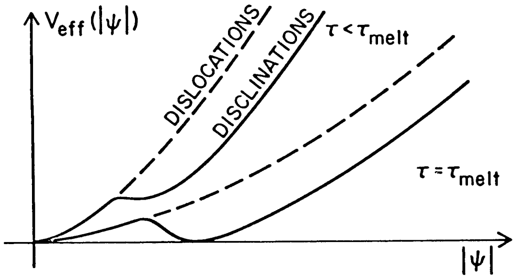

Fig. 1. The effective energy of the transverse dislocation field. Above $|\psi_c|$, the disclinations undergo a pair unbinding transition. At sufficiently high temperature (low curvature) this leads to a first order transition.

At the mean-field level, the dislocations by themselves have an effective potential

$$V_{\text{eff}}(|\psi|) = \sum_l \{[(E^{\text{T}} + \tfrac{1}{2}\pi)/\pi t - \tfrac{1}{4}]\,|\psi_l|^2 + \tfrac{1}{64}|\psi_l|^4 + ...\}, \tag{12}$$

which shows that they proliferate in a continuous phase transition at $t_c = (4/\pi)(E^{\text{T}} + \frac{1}{2}\pi)$. We shall now demonstrate that the nature of the transition is changed drastically by the possibility of unbinding disclinations: For $|\psi| \neq 0$, the $\phi(x)$ field has a new correlation function in which $v_4(x)$ is modified to

$$\tilde{v}_4(x) = \sum_k \exp(ikx)\,\frac{1}{K^4 + (\pi/2t)|\psi|^2 K^2} = \frac{1}{(\pi/2t)|\psi|^2}\sum_k \exp(ikx)\left(\frac{1}{K^2} - \frac{1}{K^2 + (\pi/2t)|\psi|^2 K''^2/K^2}\right). \tag{13}$$

The first term reproduces the conservation of disclination changes. Following the same subtraction procedure as for $v_2(x)$, we arrive at the following disclination sum m

$$\sum_{m(x)} \delta_{\Sigma_x m,0} \exp\{E'/t + (4/|\psi|^2)[\tfrac{1}{4} + v_2^{|\psi|}(0)]\}$$

$$\times \sum_x m^2 \exp\left(-\frac{4}{|\psi|^2}\sum_{x\neq x'}'' m(x)[v_2''(x-x') - v_2^{|\psi|}(x-x')]\,m(x')\right), \tag{14}$$

where $v_2^{|\psi|}(x)$ is the short-range Yukawa lattice potential

$$v_2^{|\psi|}(x) \equiv \sum_k \exp(ikx)\,\frac{1}{K^2 + (\pi/2t)|\psi|^2}\,. \tag{15}$$

For small $|\psi|$, the potential is so strongly attractive and the core energy so large that disclinations cannot appear. As $|\psi|$ increases, the Coulomb part $v_2''(x)$ in (13) has a Kosterlitz–Thouless phase transition with dislocations proliferating fro $|\psi|^2 > 1/\pi$. Above that point there is additional entropy which changes the effective potential qualitatively in the way shown in fig. 1. This always leads to a first order transition of a temperature t_{melt} below the critical value t_c [see (12)] at which the dislocations would have proliferated by themselves. Thus it is the opening up of this otherwise completely closed set of degrees of freedom which is responsible for the first order of the transition.

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