DUAL MODEL FOR DISLOCATION AND DISCLINATION MELTING

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We show that defect melting involving dislocations and disclinations is dually equivalent to an extension of an XY model with an energy of the type $\Sigma_{i,j}\{[\cos(\nabla_i u_j + \nabla_j u_i) + \epsilon \cos \nabla_i \omega_j]\}$, where $\omega_i = \frac{1}{2}\epsilon_{ijk}\nabla_j u_k$ is the local rotation field. The model clarifies the proper choice of defect core energies arising from nonlinear elasticity. These permit the pile-up of dislocations to disclinations which is essential for the first order of the melting transition.

Recently, it has become clear that simple proliferation of dislocation lines alone is not sufficient for understanding the melting transition but that disclination lines are responsible for making the transition first order [1]. The conclusions were based on mean field studies of a newly developed disorder field theory of line-like defects [‡1]. It would be desirable to verify this conclusion with Monte Carlo computer simulations. The ensemble of defect lines itself with their long-range interactions is not well suited for this purpose. A local model, which is dual to such an ensemble, is preferable. In the present note we present such a model. It is an extension of a previous model [3] which was closely related to a U(1) lattice gauge theory, in which the role played by disclinations was not clear.

At first, we shall consider two-dimensional systems. Let $\hat{u}_i$ be the atomic displacements normalized such that $\hat{u}_i = 2\pi$ amounts to a period in a simple cubic lattice. Then the elastic energy is

$$E = \frac{a^2}{(2\pi)^2}\sum_x [\tfrac{1}{4}\mu(\nabla_i\hat{u}_j + \nabla_j\hat{u}_i)^2 + \tfrac{1}{2}\lambda(\nabla_i\hat{u}_i)^2],$$

where $\nabla_i u_j(x) \equiv u_j(x+i) - u_j(x)$ are the lattice derivatives (neglecting anisotropies). Defects and their proper long-range interactions can then be studied by a nonlinear generalization of this energy in a partition function

$$Z = \prod_{x,i}\int_{-\pi}^{\pi}\frac{d\hat{u}_i(x)}{2\pi}\exp\Big(-\beta\sum_x\{[1-\cos(\nabla_1\hat{u}_2 + \nabla_2\hat{u}_1)]$$
$$+ 2(2 - \cos\nabla_1\hat{u}_1 - \cos\nabla_2\hat{u}_2) + (\lambda/\mu)[1-\cos(\nabla_1\hat{u}_1 + \nabla_2\hat{u}_2)]\}\Big), \tag{1}$$

where $\beta \equiv a^D\mu/(2\pi)^2 T$ in D dimensions. By a Villain approximation this is about equal to

$$Z = \sum_{n_{ij}(x)}\prod_{x,i}\int_{-\pi}^{\pi}\frac{d\hat{u}_i(x)}{2\pi}\exp\left\{-\beta\left[\sum_{x,i,j}\tfrac{1}{4}(\nabla_i\hat{u}_j + \nabla_j\hat{u}_i - 2\pi n_{ij})^2 + \frac{\lambda}{2\mu}\sum_x\Big(\sum_i(\nabla_i\hat{u}_i - \pi n_{ii})\Big)^2\right]\right\}, \tag{2}$$

‡1 For the developments leading up to this field theory see ref. [2].

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where the sum over integer $n_{ij} (n \neq j)$ and even n_{ii} accounts for periodic jumps of atoms. Stresses are introduced via a quadratic completion

$$Z = \sum_{n_{ij}(x)} \prod_{x,i} \int_{-\pi}^{\pi} \frac{d\hat{u}_i}{2\pi} \prod_{x,i>j} \int_{-\infty}^{\infty} \frac{d\hat{\sigma}_{ij}(x)}{\sqrt{2\pi\beta}} \exp\left[-\frac{1}{4\beta}\sum_{x,i,j}\left(\hat{\sigma}_{ij}^2 - \frac{\nu}{1+\nu}\hat{\sigma}_{ii}^2\right)\right] \exp\left(\frac{i}{2}\sum_{x,i,j}\hat{\sigma}_{ij}(\nabla_i\hat{u}_j + \nabla_j\hat{u}_i - 2\pi n_{ij})\right), \quad (3)$$

where $\nu \equiv \lambda/[(D-1)\lambda + 2\mu]$ is the Poisson number in D dimensions. The sum over n_{ij} makes $\hat{\sigma}_{ij}$ integer, say $\bar{\sigma}_{ij}$, and the integrals over $\hat{u}_i$ enforce $\nabla_i \bar{\sigma}_{ij} = 0$. The normalization factor between $\hat{\sigma}_{ij}$ and the proper stresses is $\bar{\sigma}_{ij}/\sigma_{ij} = a^D/2\pi T$. The defects in ref. [3] arose by rewriting $\bar{\sigma}_{ij} = \epsilon_{ik}\nabla_k \bar{A}_j$ with $\nabla_j \bar{A}_j = 0$, and enforcing the integerness of $\bar{A}_j$ via an integer transverse vector field $b_i^{\mathrm{T}}(x)$ with $\bar{\nabla}_i b_i^{\mathrm{T}}(x) = 0$, with a partition function

$$Z = \prod_{x,i} \int \frac{dA_i(x)}{2\pi} \delta(\nabla_i A_i) \exp \sum_x \left(-\frac{1}{4\beta'}[\nabla_i A_j(x)]^2 + 2\pi i A_i(x)\, b_i^{\mathrm{T}}(x)\right), \quad (4)$$

where $\beta \equiv a^2\mu'/(2\pi)^2 T$ with $\mu' = (1+\nu)\mu$. This is not, however, the model which leads to the first-order phase transition. Disclination sources are missing. In order to enter them into the partition function (1) we have to keep in mind that disclinations are very singular objects, quite similar to pinholes. It is well known that close to such objects, the linear approximation to elasticity is quite bad. Thus the elastic energy requires inclusion of a term $f = [a^2\mu/(2\pi)^2]\, \epsilon(\partial_i\hat{\omega})^2$ where $\hat{\omega} = \frac{1}{2}(\partial_1\hat{u}_2 - \partial_2\hat{u}_1)$ is the local rotation field. There exists a simple nonlinear generalization of this energy which produces disclinations. Let us recall that the dislocation density is define differentially by the lack of derivatives to commute in front of the displacement field $\bar{\alpha}_j = (1/2\pi)\epsilon_{kl}\partial_k\partial_l\hat{u}_j$. The disclination density has a similar definition with respect to the rotation field $\hat{\omega}$: $\bar{\Theta} = (1/2\pi)\epsilon_{kl}\partial_k\partial_l\hat{\omega}$. Actually, these definitions hold only in the continuum limit. Otherwise disclinations are more complicated objects. We shall neglect these complications and treat disclinations in the differential approximation, multiplying the partition function (1), (2) by a factor, under the integral,

$$\exp\left(-\beta\sum_{x,i}[1-\cos(\nabla_i\hat{\omega})]\right) \sim \sum_{m_i(x)} \exp\left(-\tfrac{1}{2}\beta\sum_{x,i}(\nabla_i\hat{\omega} - 2\pi m_i)^2\right).$$

The new energy can be brought to a canonical form of type (3) by introducing the rotational stresses $\hat{\pi}_i$ and writing

$$Z = \sum_{n_{ij}(x)}\sum_{m_i(x)} \int_{-\pi}^{\pi}\frac{d\hat{u}_i}{2\pi}\prod_{x,i,j}\int_{-\infty}^{\infty}\frac{d\hat{\sigma}_{ij}}{\sqrt{2\pi\beta}}\prod_{x,i}\int_{-\pi}^{\pi}\frac{d\hat{\omega}_i}{2\pi}\int\frac{d\hat{\pi}_i}{\sqrt{2\pi\beta}}\exp\left\{-\frac{1}{4\beta}\left[\sum_x\left(\hat{\sigma}_{s,ij}^2 - \frac{\nu}{1+\nu}\hat{\sigma}_{s,ii}^2\right) + \epsilon^{-1}\pi_i^2\right]\right\}$$

$$\times \exp\left(\frac{i}{2}\sum_{x,i,j}\hat{\sigma}_{ij}(\nabla_j\hat{u}_i - 2\pi n_{ij} - \epsilon_{ji}\hat{\omega}) + i\sum_{x,i}\hat{\pi}_i(\partial_i\hat{\omega} - 2\pi m_i)\right), \quad (5)$$

where $\hat{\sigma}_{s,ij}$ is the symmetric part of the stress tensor. The sums over n_{ij} and m_i make $\hat{\sigma}_{ij}$, $\hat{\pi}_i$ integer, say $\bar{\sigma}_{ij}$, $\bar{\pi}_i$, and the integrals over $\hat{u}$ and $\hat{\omega}$ enforce

$$\nabla_j\bar{\sigma}_{ij} = 0, \quad \nabla_j\bar{\pi}_j = \epsilon_{ij}\bar{\sigma}_{ij}, \quad (6)$$

which are the two-dimensional versions of the well-known conservation laws for stress and rotation stress (following from the fact that σ_{ij} and π_i are momentum and angular momentum densities of the displacement field u_i). The stress energy involves only the symmetric part of the stress tensor such that the integration over the antisymmetric part of $\hat{\sigma}_{ij}$ enforces the identity $\omega \equiv \frac{1}{2}(\nabla_1 u_2 - \nabla_2 u_1)$. We now introduce fields A_i and h which guarantee (6):

$$\bar{\sigma}_{ij} = \epsilon_{jk}\nabla_k A_i, \quad \bar{\pi}_i = \epsilon_{ik}\nabla_k h - A_i, \quad (7)$$

and keep $\bar{\sigma}_{ij}$, $\bar{\pi}_i$ integer via a defect sum

$$\sum_{b_i(x)} \sum_{m(x)} \exp\left[2\pi i\left(\sum_x b_i(x) A_i(x) + m(x)\, h(x)\right)\right]. \tag{8}$$

Since the energy depends only on the symmetric part of stress, the longitudinal part of A_i is really decoupled and we arrive at a partition function

$$Z = \sum_{m(x)} \sum_{b_i^{\mathrm{T}}} \prod_{x,i} \int \frac{\mathrm{d}A_i(x)}{\sqrt{2\pi\beta'}} \delta(\nabla_i A_i) \prod_x \int \frac{\mathrm{d}h(x)}{\sqrt{2\pi\beta\epsilon}} \exp \sum_x \left[-\frac{1}{4\beta'}\left((\nabla_i A_j)^2 + \frac{1+\nu}{\epsilon}(\epsilon_{ik}\nabla_k h - A_i)^2\right)\right.$$
$$\left. + 2\pi i[b_i^{\mathrm{T}}(x) A_i(x) + m(x) h(x)]\right]. \tag{9}$$

This is the type of partition function for which a first-order melting transition was established in ref. [1].

The nonlinearities of the interactions are included in the second term. For $\epsilon \to 0$, the field A_i is squeezed against $\epsilon_{ik}\nabla_k h$ and the disclinations decouple, forming a trivial, albeit infinite, overall factor. Then the transition is continuous. For $\epsilon \neq 0$, however, the disclinations enhance the proliferation of $b_i^{\mathrm{T}}(x)$ configurations at a certain temperature and it is this process which makes the transition first order.

Notice that the disclinations can be combined with the transverse dislocations to write Z in the form

$$Z = \sum_{m(x)} \sum_{b_i(x)} \prod_{x,i} \int \frac{\mathrm{d}A_i(x)}{\sqrt{2\pi\beta'}} \delta(\nabla_i A_i) \exp \sum_x \left(-\frac{1}{4\beta'}(\nabla_i A_j)^2 + 2\pi i b_i(x) A_i(x) - 4\pi^2\beta\epsilon m(-\nabla^2)^{-1} m\right), \tag{10}$$

where

$$b_i = b_i^{\mathrm{T}} + \delta_{i2} \sum_{x_1'=-\infty}^{x_1} m(x_1', x_2)$$

is now an unconstrained field of integer Burgers' vectors. Actually, this decomposition is not unique. We can choose a unit vector $\boldsymbol{e}$ along the $\boldsymbol{x}$ or $\boldsymbol{y}$ direction and define $b_i = b_i^{\mathrm{T}} - (1/\boldsymbol{e}\cdot\nabla)\,\epsilon_{ik} e_k m$. This way of writing our model exhibits quite clearly the difference with respect to other constructions [5] which undergo a continuous transition. There is no ad hoc core energy $\propto b_i^2$, which would forbid the pile-up of strings of dislocations to form a disclination. The additional energy $m(-\nabla^2)^{-1} m$ which here is *derived* from the nonlinearities of the forces, *does* allow for this pile-up which drives the transition first order.

Our considerations can easily be extended to three dimensions where we add $f = a^2\mu(2\pi)^{-2}\epsilon[\frac{1}{2}(\partial_i\omega_j + \partial_j\omega_i)]^2$ and the exponent (5) becomes

$$\sum_x \left(-\tfrac{1}{4}\beta\{\bar{\sigma}_{\mathrm{s},ij}^2 - [\nu/(1+\nu)]\,\bar{\sigma}_{\mathrm{s},ii}^2\} + i\sigma_{ij}(\nabla_j u_i - \epsilon_{jik}\omega_k - 2\pi n_{ji}) - (\beta/4\epsilon)\,\bar{\pi}_{\mathrm{s},ij}^2 + i\bar{\pi}_{ij}(\nabla_j\omega_i - 2\pi m_{ji})\right), \tag{11}$$

leading to integer stresses and rotational stresses with the conservation laws

$$\bar{\nabla}_i\bar{\sigma}_{ij} = 0, \quad \bar{\nabla}_j\bar{\pi}_{ij} = \epsilon_{ikl}\bar{\sigma}_{kl}. \tag{12}$$

These can be enforced by introducing gauge fields

$$\bar{\sigma}_{ij} = \epsilon_{jkl}\bar{\nabla}_k A_{li}, \quad \bar{\pi}_{ij} = \epsilon_{jkl}\bar{\nabla}_k h_{li} + \delta_{ij} A_{li} - A_{ij}, \tag{13}$$

with the gauge invariance

‡2 For a discussion of these conservation laws see ref. [6]. The symmetry between the conservation laws of defects in (15) and those of stresses (6) is further developed in ref. [7].

$$\bar{A}_{li} \to \bar{A}_{li} + \nabla_l \Lambda_i, \quad \bar{h}_{li} \to \bar{h}_{li} - \epsilon_{lik}\Lambda_k, \quad \bar{h}_{li} \to h_{li} + \nabla_l \xi_i, \tag{14}$$

which are made integer by the following integer defect sums

$$\sum_{\bar{a}_{ij}\Theta_{ij}} \delta_{\nabla_j \bar{a}_{ij}, \epsilon_{ikl}\bar{\Theta}_{kl}} \delta_{\nabla_j \bar{\Theta}_{ji},0} \exp\left(2\pi\mathrm{i} \sum_{x,ij} (\bar{a}_{ij} A_{ji} + \Theta_{ij} h_{ji})\right). \tag{15}$$

The δ-functions ensure the well-known conservation laws of defect densities and we see that the gauge degrees of freedom are properly decoupled.

Since the elastic energy does not involve the antisymmetric parts of σ_{ij}, π_{ij} it depends only on those parts of A_{ij}, h_{ij} which have $\nabla_i A_{ji} - \nabla_j A_{ii} = 0$, $\nabla_i h_{ji} - \nabla_j h_{ii} = -\epsilon'_{jkl} A_{kl}$. In order to avoid an infinite overall factor we must restrict the defect sum to a constraint subset, say $\alpha^{\mathrm{c}}_{ij}, \Theta^{\mathrm{c}}_{ij}$ of α_{ij}, Θ_{ij} configurations which satisfy, in addition to the conservation laws in (15),

$$\bar{\nabla}_i \alpha^{\mathrm{c}}_{ij} - \bar{\nabla}_j \alpha^{\mathrm{c}}_{ii} = 0, \quad \bar{\nabla}_i \Theta^{\mathrm{c}}_{ij} - \bar{\nabla}_j \Theta^{\mathrm{c}}_{ii} = -\epsilon_{jkl}\alpha_{lk}. \tag{16}$$

In terms of helicity amplitudes $\alpha^{(l,m)}$, this forces α^{c}_{ij} to contain only (2, 2), (2, −2), (1, 0) components, while Θ^{c}_{ij} has, in addition, a component $\propto (1/\sqrt{3})[(2,0) - \sqrt{2}(0,0)]$ which, however, is proportional to the (1, 0) component of α^{c}_{ij} [3].

It is useful to introduce the symmetric tensor gauge field χ_{ql} via $A_{li} \equiv \epsilon_{ipq} \nabla_p \chi_{ql}$. Then

$$\bar{\sigma}_{ij} = \epsilon_{ipq}\epsilon_{jkl} \bar{\nabla}_p \bar{\nabla}_k \chi_{ql}, \quad \bar{\pi}_{ij} = \epsilon_{jkl} \bar{\nabla}_k h'_{li}, \quad \nabla_i h'_{jl} - \nabla_j k'_{ii} = 0, \tag{17}$$

where $h'_{li} \equiv h_{li} - \chi_{li}$ and the coupling (15) to defects becomes simply

$$\exp\left(2\pi\mathrm{i} \sum_{x,ij} (\bar{\eta}_{ij}\chi_{ji} + \bar{\Theta}^{\mathrm{c}}_{ij} h'_{ji})\right), \tag{18}$$

where

$$\bar{\eta}_{ij} = \bar{\Theta}^{\mathrm{c}}_{ij} - \tfrac{1}{2}\bar{\nabla}_m [\epsilon_{mjl}\bar{\alpha}^{\mathrm{c}}_{li} + (i \to j) + \epsilon_{ijl}\bar{\alpha}^{\mathrm{c}}_{lm}]$$

is the symmetric defect density. The path integrals over χ and h' are now independent, the latter producing an extra ϵ/R interaction energy between the (2, 2), (2, −2), (1, 0) components of disclinations. As compared with the R energy caused by the χ field, this is "short-range". When dislocations proliferate, the $1/R$ interaction is screened to a δ-function, thus producing merely an extra core energy of disclinations.

The present model differs from the one treated in ref. [1] by the restrictions (16) imposed upon the defect lines. Nevertheless, a study of the disorder field theory associated with these restricted lines suggests again a first-order phase transition, albeit with a smaller entropy jump. This is, in fact, desirable, since that in ref. [1] was too large ($\Delta S/R \sim 2.4$) as compared with experiment ($\Delta S/R \sim 1.4$).

Just as in the two-dimensional case, the disclination density Θ^{c}_{ij} can be absorbed into the dislocation density forming

$$\alpha_{ij} = \alpha^{\mathrm{c}}_{ij} - (1/\boldsymbol{e}\cdot\nabla)\,\epsilon_{ikl} e_k \Theta^{\mathrm{c}}_{jl},$$

where the unit vector $\boldsymbol{e}$ can point in $\boldsymbol{x}, \boldsymbol{y}$, or $\boldsymbol{z}$ direction. This tensor comprises all 6 components satisfying $\bar{\nabla}_j \alpha_{ij} = 0$. It can be used to express the interaction in the form

$$\exp\left(2\pi\mathrm{i} \sum_{\boldsymbol{x},i,j} (\alpha_{ij} A_{ij} + \Theta^{\mathrm{c}}_{ij} h'_{ij})\right),$$

with the h'_{ij} integral producing again an ϵ/R interaction energy for the disclination content in α_{ij}. This properly allows for the pile-up of sheets of dislocations to disclinations which is essential for the first order of the melting transition.

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