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Defect-mediated melting of pentagonal quasicrystals

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Abstract. The theories of dislocation- and disclination-mediated melting in two-dimensional systems, due to Kosterlitz, Thouless, Nelson, Halperin and Young, are applied to pentagonal quasicrystals. As in triangular lattices, the transition from solid to liquid occurs in two stages. First, dissociation of neutral pairs of dislocations causes a transition out of the low-temperature solid phase, which is characterised by algebraically decaying quasiperiodic translational order and long-range fivefold orientational order, into a 'pentahedratic' phase with exponentially decaying translational order and algebraically decaying orientational order. A second transition, caused by dissociation of pairs of disclinations, leads to an isotropic fluid whereby orientational order also decays exponentially. We present the relevant recusion relations and critical exponents.

1. Introduction

Quasicrystals are characterised by the presence of both quasiperiodic translational order and bond-orientational order (the latter associated with a non-crystallographic point group). As in conventional crystals, the destruction of these types of long-range order can occur through the generation of isolated topological defects. Specifically, dislocations destroy the translational order, while disclinations destroy the bond-orientational order. In a two-dimensional quasicrystal, an analytic study of its melting via the generation of defects can be carried out, in much the same way as was done for conventional crystals by Kosterlitz, Thouless, Nelson, Halperin and Young (Kosterlitz and Thouless 1973, Nelson and Halperin 1979, Young 1979). In this paper we carry out this study for the case of pentagonal quasicrystals assuming that the phason field has reached equilibrium. For a discussion of the dynamics of the phason field see, e.g., Lubensky *et al* (1985) and Frenkel *et al* (1986). We find that melting occurs in two stages, as in the conventional case. Upon dissociation of neutral pairs of dislocations, the quasicrystal melts into a 'pentahedratic' phase with exponentially decaying translational order and algebraically decaying orientational order. A subsequent transition at higher temperature completes the melting into the liquid phase.

Our analysis is based on the harmonic elastic energy density of a pentagonal quasicrystal (Levine *et al* 1985, Bak 1985)

$$f_{\mathrm{el}} = \tfrac{1}{2}\lambda u_{ii}u_{ii} + \mu u_{ij}u_{ij} + \tfrac{1}{2}K_1 w_{ij}w_{ij} + K_2(w_{xx}w_{yy} - w_{yx}w_{xy}) + K_3[(u_{xx} - u_{yy})(w_{xx} + w_{yy}) + 2u_{xy}(w_{xy} - w_{yx})] \qquad (1.1)$$

where $u_{ij} = \frac{1}{2}(\partial u_i/\partial x_j + \partial u_j/\partial x_i)$ and $w_{ij} = \partial w_i/\partial x_j$. The fields $\boldsymbol{u}(\boldsymbol{r})$ and $\boldsymbol{w}(\boldsymbol{r})$ are the phonon and phason fields, respectively, which characterise the hydrodynamic modes of the quasicrystal. In terms of these fields we can give a continuum description of the mass density $\rho(\boldsymbol{r})$ of the quasicrystal by writing

$$\rho(\boldsymbol{r}) = \sum_{\boldsymbol{G}_n} \rho_{\boldsymbol{G}_n}(\boldsymbol{r}) \exp(\mathrm{i}\boldsymbol{G}_n \cdot \boldsymbol{r}) \tag{1.2a}$$

$$\rho_{\boldsymbol{G}_n}(\boldsymbol{r}) = |\rho_{\boldsymbol{G}_n}| \exp(\mathrm{i}\boldsymbol{G}_n \cdot \boldsymbol{u}(\boldsymbol{r}) + \mathrm{i}\boldsymbol{G}_{\langle 3n\rangle_5} \cdot \boldsymbol{w}(\boldsymbol{r})) \tag{1.2b}$$

where the reciprocal lattice vectors $\boldsymbol{G}_n$ are given by

$$\boldsymbol{G}_n = G\left(\cos\frac{2\pi n}{5}, \sin\frac{2\pi n}{5}\right) \qquad n = 0, 1, \ldots 4 \tag{1.3}$$

and their reflections. The symbol $\langle 3n\rangle_5$ denotes $3n \bmod 5$.

The presence of quasiperiodic translational order can be assessed via the Debye-Waller correlation function:

$$C_G(\boldsymbol{r}) = \langle \rho_G(\boldsymbol{r}) \rho_G^*(0) \rangle. \tag{1.4}$$

In a three-dimensional quasicrystal, this would tend to a finite value as $r \to \infty$; in two dimensions at low temperatures, as in conventional solids, C_G decays algebraically. Specifically

$$C_G(\boldsymbol{r}) \sim r^{-\eta_G} \tag{1.5a}$$

where

$$\eta_G = \frac{|\boldsymbol{G}|^2 k_{\mathrm{B}} T}{4\pi[(2\mu+\lambda)K_1 - K_3^2](\mu K_1 - K_3^2)} \{[(2\mu+\lambda)K_1 - K_3^2](K_1 + \mu\tau^2) + (\mu K_1 - K_3^2)[K_1 + (2\mu+\lambda)\tau^2]\} \tag{1.5b}$$

and τ is the golden mean. We obtained this result by evaluating (1.4) in the harmonic approximation (1.1) and neglecting dislocations and disclinations.

Long-range orientational order (fivefold or, equivalently, tenfold in the present case) can be characterised in terms of the behaviour of the orientational correlation function:

$$C_\theta(\boldsymbol{r}) = \langle \psi(\boldsymbol{r}) \psi^*(\boldsymbol{0}) \rangle \tag{1.6a}$$

where

$$\psi(\boldsymbol{r}) = \exp(10\mathrm{i}\theta(\boldsymbol{r})) \tag{1.6b}$$

and,

$$\theta(\boldsymbol{r}) = \frac{1}{2}\left(\frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y}\right). \tag{1.6c}$$

As we show in § 3, C_θ approaches a constant at large $\boldsymbol{r}$, in the low-temperature phase where only bound dislocations and disclinations exist.

In the remainder of this paper we consider the melting of the pentagonal quasicrystal, first (§ 2) into the 'pentahedratic' phase characterised by $C_G(\boldsymbol{r}) \sim \exp(-r/\xi)$ and $C_\theta(\boldsymbol{r}) \sim r^{-\eta_{10}}$, and subsequently into the liquid phase (§ 3).

2. Dislocation-unbinding transition

2.1. Recursion relations

In the presence of dislocations, the total harmonic energy of an elastic medium can be written as a sum of two parts:

$$H_{\mathrm{E}} = H_0 + H_{\mathrm{D}} \tag{2.1}$$

where H_0 is the energy due to the smoothly varying long-wavelength phonon and phason modes (i.e. of the form (1.1)), and H_{D} is the energy due to the dislocations. Since the low-temperature solid phase is characterised by dislocations that only occur as neutral pairs, we consider a charge neutral distribution of dislocations such that

$$\int \mathrm{d}^2 r\, \boldsymbol{b}(\boldsymbol{r}) = 0.$$

Written in terms of $\tilde{u}^{\mathrm{b}}_{ij}$, which are the components of the 8-vector whose first four components are the four smooth, or bare, phonon strains u^{b}_{ij} and the last four are the bare phason strains, H_0 is of the form (De and Pelcovits 1987a)

$$\frac{H_0}{k_{\mathrm{B}}T} = \frac{1}{2}\int \frac{\mathrm{d}^2 r}{a_0^2}\, \tilde{u}^{\mathrm{b}}_{ij}\tilde{\phi}_{ijkl}\tilde{u}^{\mathrm{b}}_{kl} \tag{2.2}$$

where a_0 is the minimum separation of the underlying lattice points and $\tilde{\phi}_{ijkl}$ are the elements of an eight-rank elastic modulus tensor which we write as

$$\phi = \begin{pmatrix} \vec{A}' & \vec{B}' \\ \vec{C}' & \vec{D}' \end{pmatrix} \tag{2.3a}$$

where $\vec{A}'$, $\vec{B}'$, $\vec{C}'$, and $\vec{D}'$ are

$$A'_{ijkl} = \bar{\lambda}\delta_{ij}\delta_{kl} + \bar{\mu}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \tag{2.3b}$$

$$B'_{ijkl} = \bar{K}_3(\delta_{i1} - \delta_{i2})(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}) \tag{2.3c}$$

$$C'_{ijkl} = \bar{K}_3(\delta_{k1} - \delta_{k2})(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}) \tag{2.3d}$$

$$D'_{ijkl} = \bar{K}_1\delta_{ik}\delta_{jl} + \bar{K}_2(\delta_{ij}\delta_{kl} - \delta_{il}\delta_{jk}) \tag{2.3e}$$

and $\bar{\mu}$, $\bar{\lambda}$, $\bar{K}_1$, $\bar{K}_2$ and $\bar{K}_3$ are dimensionless quantities which equal the corresponding elastic constants multiplied by a_0^2 and divided by $k_{\mathrm{B}}T$.

The dislocation contribution H_{D} to the total elastic energy in (2.1) can be written as a sum over all neutral pairs of dislocations. For the general expression for the interaction energy of an arbitrary but charge-neutral distribution of dislocations in pentagonal quasicrystals, we refer the reader to our earlier work (De and Pelcovits 1987a). Applying the general result to a neutral pair of dislocations separated by $\boldsymbol{R} = R(\sin\theta, \cos\theta)$, with Burgers' vectors $\pm\tilde{\boldsymbol{b}}_n = \pm(\boldsymbol{b}_n \oplus \boldsymbol{d}_n)$ where (Levine *et al* 1985)

$$b_n = R\left(-\sin\frac{2\pi n}{5}, \cos\frac{2\pi n}{5}\right) \qquad d_n = R\left(-\sin\frac{2\pi\langle 3n\rangle_5}{5}, \cos\frac{2\pi\langle 3n\rangle_5}{5}\right) \tag{2.4}$$

we find that their interaction energy is

$$\begin{aligned} H^n_{\mathrm{D}} = \frac{1}{4\pi}\Bigg\{ & M\left(\boldsymbol{b}_n\cdot\boldsymbol{b}_n \ln\frac{R}{a} - \frac{(\boldsymbol{b}_n\cdot\boldsymbol{R})^2}{R^2}\right) + N\boldsymbol{d}_n\cdot\boldsymbol{d}_n \ln\frac{R}{a} \\ & + W\left(\frac{R_x(R_x^2 - 3R_y^2)}{R^3}\, d_{n,x} + \frac{R_y(3R_x^2 - R_y^2)}{R^3}\, d_{n,y}\right)^2 \\ & + S\left[\frac{1}{4}\,\frac{R_x^2 - R_y^2}{R^2}\,\boldsymbol{b}_n\cdot\boldsymbol{d}_n + \frac{1}{2}\,\frac{R_xR_y}{R^2}\,\varepsilon_{ij}b_{n,i}d_{n,j}\right. \\ & \left. + \frac{1}{2}\,\frac{\boldsymbol{b}_n\cdot\boldsymbol{R}}{R}\left(\frac{R_x(R_x^2 - 3R_y^2)}{R^3}\, d_{n,x} + \frac{R_y(3R_x^2 - R_y^2)}{R^3}\, d_{n,y}\right)\right]\Bigg\} - 2\ln y \end{aligned} \tag{2.5a}$$

where

$$M=\frac{4(\mu+\lambda)(\mu K_1-K_3^2)}{(2\mu+\lambda)K_1-K_3^2} \tag{2.5b}$$

$$N=2K_1+\frac{2K_3^2(2K_2-K_1)}{(2\mu+\lambda)K_1-K_3^2}+\frac{(\mu+\lambda)K_1K_3^2(2K_2-K_1)}{(\mu K_1-K_3^2)[(2\mu+\lambda)K_1-K_3^2]} \tag{2.5c}$$

$$W=\frac{(\mu+\lambda)K_1K_3^2(2K_2-K_1)}{3(\mu K_1-K_3^2)[(2\mu+\lambda)K_1-K_3^2]} \tag{2.5d}$$

$$S=\frac{4(\mu+\lambda)K_3(K_2-K_1)}{(2\mu+\lambda)K_1-K_3^2} \tag{2.5e}$$

and y is the probability of finding a neutral pair of dislocations whose separation is a_0, i.e.

$$y=\exp(-E_c a_0^2/k_B T) \tag{2.5f}$$

where E_c is the core energy of a dislocation.

The effect of dislocations in any elastic medium is to renormalise the bare elastic constants. Physically this corresponds to successive screening of pairs with large separations by pairs with smaller separations, thus leading to weaker elastic constants. Mathematically, renormalisation then implies that, in the presence of bound dislocations, the total elastic energy H_E has the same form as H_0 in (2.2), except that the bare strain is replaced by the total strain $\tilde{u}_{ij}=\tilde{u}_{ij}^b+\tilde{u}_{ij}^s$, where $\tilde{u}_{ij}^s$ is the singular strain due to dislocations (De and Pelcovits 1987a). Also the bare elastic tensor $\tilde{\phi}_{ijkl}$ is replaced by the renormalised elastic tensor $\tilde{\phi}_R$.

The renormalised tensor $\tilde{\phi}_R$ is the best determined in terms of its inverse, whose components are related to correlation functions of the total strains:

$$\tilde{\phi}_{R,ijkl}^{-1}=\frac{1}{\Omega a_0^2}\langle \tilde{U}_{ij}\tilde{U}_{kl}\rangle_{H_E} \tag{2.6}$$

where Ω is the area and

$$\tilde{U}_{ij}=\int d^2r\,\tilde{u}_{ij}(\boldsymbol{r}). \tag{2.7}$$

The subscript H_E on the average indicates that the average is performed over the distribution $\exp(-\beta H_E)$. Due to charge neutrality $\langle \tilde{U}_{ij}^b\tilde{U}_{kl}^b\rangle_{H_D}=\langle \tilde{U}_{ij}^s\tilde{U}_{kl}^s\rangle_{H_0}=\langle \tilde{U}_{ij}^s\tilde{U}_{kl}^b\rangle_{H_D}=0$. So we can rewrite (2.5) as

$$\tilde{\phi}_{R,ijkl}^{-1}=\tilde{\phi}_{ijkl}^{-1}+\frac{1}{\Omega a_0^2}\langle \tilde{U}_{ij}^s\tilde{U}_{kl}^s\rangle_{H_D} \tag{2.8}$$

where $\tilde{\phi}_{ijkl}^{-1}$ is the inverse of the bare elastic tensor. Explicitly, the components $\tilde{\phi}_{ijkl}^{-1}$ can be expressed as

$$\tilde{\phi}^{-1}=\begin{pmatrix}\tilde{A} & \tilde{B}\\ \tilde{C} & \tilde{D}\end{pmatrix} \tag{2.9a}$$

where the tensors $\tilde{A}$, $\tilde{B}$, $\tilde{C}$ and $\tilde{D}$ are

$$A_{ijkl}=-\left(\frac{\bar{\lambda}}{4\bar{\mu}(\bar{\mu}+\bar{\lambda})}+\frac{\bar{K}_3^2}{2\bar{\mu}[\bar{\mu}(\bar{K}_1+\bar{K}_2)-2\bar{K}_3^2]}\right)\delta_{ij}\delta_{kl}$$
$$+\left(\frac{1}{4\bar{\mu}}+\frac{\bar{K}_3^2}{2\bar{\mu}[\bar{\mu}(\bar{K}_1+\bar{K}_2)-2\bar{K}_3^2]}\right)(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}) \tag{2.9b}$$

$$B_{ijkl} = -\frac{\bar{K}_3}{2[\bar{\mu}(\bar{K}_1+\bar{K}_2)-2\bar{K}_3^2]}(\delta_{i1}-\delta_{i2})(\delta_{ij}M\delta_{kl}+\delta_{ik}\delta_{jl}-\delta_{il}\delta_{jk}) \quad (2.9c)$$

$$C_{ijkl} = -\frac{\bar{K}_3}{2[\bar{\mu}(\bar{K}_1+\bar{K}_2)-2\bar{K}_3^2]}(\delta_{k1}-\delta_{k2})(\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}-\delta_{il}\delta_{jk}) \quad (2.9d)$$

$$D_{ijkl} = \frac{\bar{\mu}(\bar{\mu}\bar{K}_1-\bar{K}_3^2)}{(\bar{\mu}\bar{K}_1-\bar{K}_3^2)^2-(\bar{\mu}\bar{K}_2-\bar{K}_3^2)^2}\delta_{ik}\delta_{jl} - \frac{\bar{\mu}(\bar{\mu}\bar{K}_2-\bar{K}_3^2)}{(\bar{\mu}\bar{K}_1-\bar{K}_3^2)^2-(\bar{\mu}\bar{K}_2-\bar{K}_3^2)^2}(\delta_{ij}\delta_{kl}-\delta_{il}\delta_{jk}). \quad (2.9e)$$

The components of the renormalised inverse tenor $\tilde{\phi}^{-1}_{\mathrm{R},ijkl}$ will have the same form as $\tilde{\phi}^{-1}_{ijkl}$ with all elastic constants replaced by their renormalised values. The difference between the renormalised and the bare values comes from the second term in (2.7), i.e. from the correlation of the singular strains due to interaction of the dislocations.

Dislocations in quasicrystals are characterised by multivalued phonon and phason fields which satisfy

$$\oint \mathrm{d}\boldsymbol{u} = \boldsymbol{b} \qquad \oint \mathrm{d}\boldsymbol{w} = \boldsymbol{d} \quad (2.10)$$

where the closed loop integration is performed around the core of the dislocation. One can construct solutions for $\boldsymbol{u}(\boldsymbol{r})$ and $\boldsymbol{w}(\boldsymbol{r})$ such that the discontinuous changes in these values occur across a cutline, along which the strains will be singular. Interpreting these singular strains over all space, we find that $\tilde{U}^{\mathrm{s}}_{ij}$ will have components (De and Pelcovits 1987a)

$$U^{\mathrm{s}}_{ij} = \int \mathrm{d}^2 r\, u^{\mathrm{s}}_{ij} = \tfrac{1}{2}(b_{n,i}\varepsilon_{jm}+b_{n,j}\varepsilon_{im})R_m \quad (2.11a)$$

$$W^{\mathrm{s}}_{ij} = \int \mathrm{d}^2 r\, w^{\mathrm{s}}_{ij} = d_{n,j}\varepsilon_{im}R_m \quad (2.11b)$$

where $b_{n,i}$ and $d_{n,i}$ represent the ith, with $i=1,2$, components of the vectors defined in (2.4).

Before we perform the averages $\langle \tilde{U}_{ij}\tilde{U}_{kl}\rangle_{H_{\mathrm{D}}}$ in (2.8) over the interaction energy of an arbitrary, but charge-neutral, distribution of dislocations, we note that H_{D} contains a small parameter: the fugacity y. The minimum configuration of dislocations allowed by neutrality is a pair whose probability $\exp(-\beta H_{\mathrm{D}})$ is proportional to y^2 as is evident from (2.5a). The next possible smallest configuration is a set of five dislocations, with one each of the Burgers' vectors belonging to the primitive set of five in (2.4); the probability of such a configuration is proportional to y^5. So, to a very good approximation, we can perform the averages $\langle \tilde{U}_{ij}\tilde{U}_{kl}\rangle_{H_{\mathrm{D}}}$ over the five probabilities $\exp(-\beta H^n_{\mathrm{D}})$ of finding the five possible neutral pairs of dislocations. Substituting into (2.5a) the explicit form for $\boldsymbol{R}$, $\boldsymbol{b}_n$ and $\boldsymbol{d}_n$, we find that the probability of finding a pair with Burgers' vector $\tilde{\boldsymbol{b}}_n$ and $-\tilde{\boldsymbol{b}}_n$ at a separation $\boldsymbol{R}$ is

$$P_n(\boldsymbol{R}) \equiv \exp(-\beta H^n_{\mathrm{D}}) = y^2\left(\frac{R}{a}\right)^{(\bar{M}+\bar{N})/4\pi} \exp\left\{-\left[(-\bar{M}+9\bar{W}-3\bar{S})\cos^2\left(\theta-\frac{2\pi n}{5}\right) - 2(12\bar{W}-\bar{S})\cos^4\left(\theta-\frac{2\pi n}{5}\right)+16\bar{W}\cos^6\left(\theta-\frac{2\pi n}{5}\right)\right]\right\} \quad (2.12)$$

where $\bar{M} = Ma_0^2/k_B T$ and so on for $\bar{N}$, $\bar{W}$ and $\bar{S}$. In writing (2.12) we have ignored all multiplicative constants as they are absorbed into normalising the probabilities.

The average $\langle \tilde{U}_{ij}\tilde{U}_{kl}\rangle_{H_D}$ involves integrating $\Sigma_n\, \tilde{U}_{ij}\tilde{U}_{kl}P_n(\boldsymbol{R})$ over all values of $\boldsymbol{R}$, i.e. over all possible separations of dislocations. The angular integral is well behaved; the integral over $R = |\boldsymbol{R}|$, however, has infrared divergences. We handle these divergences by breaking up the integral into two parts (Nelson and Halperin 1979):

$$\int_a^\infty \frac{\mathrm{d}R}{a} \rightarrow \int_a^{ae^\delta} \frac{\mathrm{d}R}{a} + \int_{ae^\delta}^\infty \frac{\mathrm{d}R}{a} \tag{2.13}$$

where δ is small. The contributions from the small R are absorbed into a redefinition of the bare elastic constants in $\tilde{\phi}^{-1}_{ijkl}$. Physically, the redefinitions of the elastic constants correspond to including the effects of screening due to those pairs whose separations are less than ae^δ. Equivalently, it corresponds to increasing the core size from a to ae^δ. To complete the renormalisation group transformations, we rescale the large R integrals, so that they again range from a to ∞. The rescaling factor is absorbed into a redefinition of the fugacity y. The expression we thus find for $\tilde{\phi}^{-1}_{\mathrm{R},ijkl}$ from (2.8) has the same form as (2.8) with the redefined elastic constants replacing the bare ones in $\tilde{\phi}^{-1}_{ijkl}$. We repeat this procedure many times such that $\delta = l$, where l is a macroscopic length; each time $\tilde{\phi}^{-1}_{ijkl}(l-\delta)$ is replaced by $\tilde{\phi}^{-1}_{ijkl}(l)$ and $y(l-\delta)$ by $y(l)$ following five recursion relations for the five independent components of $\tilde{\phi}^{-1}$ (cf (2.9)) and one recursion relation for the fugacity. These relations are

$$\frac{\mathrm{d}y(l)}{\mathrm{d}l} = \left(2 - \frac{\bar{M}+\bar{N}}{8\pi}\right) y(l) \tag{2.14a}$$

$$\frac{\mathrm{d}}{\mathrm{d}l}\left(\frac{2\bar{\mu}(l)+\bar{\lambda}(l)}{4\bar{\mu}(l)[\bar{\mu}(l)+\bar{\lambda}(l)]} + \frac{\bar{K}_3^2(l)}{2\bar{\mu}(l)[\bar{\mu}(l)[\bar{K}_1(l)+\bar{K}_2(l)]-2\bar{K}_3^2(l)]}\right)$$
$$= y^2(l)[0.625P_1(l)+1.25P_2(l)] \tag{2.14b}$$

$$\frac{\mathrm{d}}{\mathrm{d}l}\left(\frac{\bar{\lambda}(l)}{4\bar{\mu}(l)[\bar{\mu}(l)+\bar{\lambda}(l)]} + \frac{\bar{K}_3^2(l)}{2\bar{\mu}(l)[\bar{\mu}(l)[\bar{K}_1(l)+\bar{K}_2(l)]-2\bar{K}_3^2(l)]}\right)$$
$$= y^2(l)[0.625P_1(l)-1.25P_2(l)] \tag{2.14c}$$

$$\frac{\mathrm{d}}{\mathrm{d}l}\left(\frac{\bar{\mu}(l)[\bar{\mu}(l)\bar{K}_1(l)-\bar{K}_3^2(l)]}{[\bar{\mu}(l)\bar{K}_1(l)-\bar{K}_3^2(l)]^2-[\bar{\mu}(l)\bar{K}_2(l)-\bar{K}_3^2(l)]^2}\right) = y^2(l)[1.25P_1(l)] \tag{2.14d}$$

$$\frac{\mathrm{d}}{\mathrm{d}l}\left(\frac{\bar{\mu}(l)[\bar{\mu}(l)\bar{K}_2(l)-\bar{K}_3^2(l)]}{[\bar{\mu}(l)\bar{K}_1(l)-\bar{K}_3^2(l)]^2-[\bar{\mu}(l)\bar{K}_2(l)-\bar{K}_3^2(l)]^2}\right) = 0 \tag{2.14e}$$

$$\frac{\mathrm{d}}{\mathrm{d}l}\left(\frac{\bar{K}_3(l)}{2[\bar{\mu}(l)[\bar{K}_1(l)+\bar{K}_2(l)]-2\bar{K}_3^2(l)]}\right) = y^2(l)[-0.625P_1(l)+1.25P_2(l)] \tag{2.14f}$$

where

$$P_1 = \int_0^{2\pi} \mathrm{d}\theta P(\theta) \qquad P_2 = \int_0^{2\pi} \mathrm{d}\theta \sin^2\theta P(\theta) \tag{2.15a}$$

with

$$P(\theta) = \exp\{-[(-\bar{M}+9\bar{W}-3\bar{S})\cos^2\theta - 2(12\bar{W}-\bar{S})\cos^4\theta + 16\bar{W}\cos^6\theta]\}. \tag{2.15b}$$

P_1 and P_2 incorporate the results of the well behaved angular integrals.

In studying (2.14) we first note that the five recursion relations for the elastic constants satisfy the stability conditions

$$\mu(l)>0 \qquad \mu(l)+\lambda(l)>0 \qquad \mu(l)K_1(l)-K_3^2(l)<0$$
$$\mu(l)K_2(l)-K_3^2(l)>0 \qquad K_1(l)-K_2(l)>0 \tag{2.16}$$

which preserve the positive-definiteness of H_E (Levine *et al* 1985). We next note that the existence of a transition is obvious from (2.14*a*). Let us recall that $y(l)$ is the probability of finding a neutral pair of dislocations whose separation is the core size ae^l. According to (2.14*a*), if $\bar{M}_R+\bar{N}_R>16\pi$, then $y(l)\to 0$ as $l\to\infty$. This characterises the solid phase where all dislocations are still in pairs with finite separations. If, however, $\bar{M}_R+\bar{N}_R<16\pi$, $y(l)\to\infty$ as $l\to\infty$; this describes the phase containing unbound dislocations. The transition temperature T_m is the temperature at which $\bar{M}_R+\bar{N}_R=16\pi$. This condition implies that, regardless of the values of the bare elastic constants, the value of the constants at T_m obey a universal constraint

$$\lim_{T\to T_m^-} M_R(T)+N_R(T)=16\pi k_B T_m/a_0^2 \tag{2.17}$$

where M_R and N_R are obtained from (2.6*b*, *c*) by replacing the bare quantities by their renormalised counterparts.

The physically measurable quantities such as $\bar{\mu}_R$ are solutions to the renormalised group equations (2.14) in the limit $l\to\infty$, i.e.

$$\bar{\mu}_R=\lim_{l\to\infty}\bar{\mu}_R(l) \tag{2.18}$$

and likewise for the remaining elastic constants. These solutions can be obtained by integrating (2.14) numerically. We find that in the solid regime, i.e. if $\bar{M}_R+\bar{N}_R>16\pi$, $y(l\to\infty)=0$. For $\bar{M}_R+\bar{N}_R<16\pi$, $y(l\to\infty)$ grows rapidly and each of the elastic constants μ_R, λ_R, K_{1R}, K_{2R} and K_{3R} approach vanishingly small constants.

2.2. *Critical exponents*

Critical exponents describe the approach of physical quantities to their values at the transition as $T\to T_m$. The manner in which the elastic constants approach their renormalised values as $T\to T_m^-$ is described by the critical exponent ν. Following arguments similar to those of Nelson and Halperin (1979) for the hexagonal lattice, it is straightforward to show that $\nu=\frac{1}{2}$. This implies that, if $\bar{\mu}^*$ is the value of $\bar{\mu}_R$ at T_m, then, as $T\to T_m^-$,

$$\bar{\mu}_R(T)=\bar{\mu}^*(1-c|t|^{1/2}) \tag{2.19}$$

where $t=(T-T_m)/T_m$ is the reduced temperature and c is a non-universal constant. That $\nu=\frac{1}{2}$ is a consequence of the fact that the recursion relations for the coupling constants are proportional to y^2 while that of the fugacity is proportional to y (Young 1979). It then follows that all the remaining elastic constants $\bar{\lambda}_R$, $\bar{K}_{1R}$, $\bar{K}_{2R}$ and $\bar{K}_{3R}$ exhibit the same cusplike singularity as in (2.19).

The critical exponent ν also characterises the behaviour of the correlation length ξ above T_m, which characterises the exponential decay of the transitional order as

$$C_G(\mathbf{r})\sim\exp(-r/\xi) \qquad T>T_m. \tag{2.20}$$

Again, using arguments similar to those in Nelson and Halperin (1979), it is straightforward to show that, as $T \to T_m^+$, the correlation length ξ diverges as

$$\xi \sim \exp(|t|^{-1/2}). \tag{2.21}$$

The behaviour of the Debye–Waller correlation function $C_G(\boldsymbol{r})$ below T_m is defined in (1.5*a*) in terms of the critical exponent η_G. As $T \to T_m^-$, we find that η_{G_n} approaches a non-universal constant:

$$\eta^*_{G_n} \equiv \lim_{T \to T_m} \eta_{G_n}(T)$$

$$= \frac{16\pi \sin^2(4\pi/5)}{25[(2\bar{\mu}^* + \bar{\lambda}^*)\bar{K}_1^* - \bar{K}_3^{*2}](\bar{\mu}^*\bar{K}_1^* - \bar{K}_3^{*2})} \times \{[(2\bar{\mu}^* + \bar{\lambda}^*)\bar{K}_1^* - \bar{K}_3^{*2}](\bar{K}_1^* + \bar{\mu}^*\tau^2) + (\bar{\mu}^*\bar{K}_1^* - \bar{K}_3^{*2}) \times [\bar{K}_1^* + (2\bar{\mu}^* + \bar{\lambda}^*)\tau^2]\} \tag{2.22}$$

where $\bar{\mu}^*$ is $\bar{\mu}_R(T_m)$ and likewise for the remaining elastic constants. We note that, unlike in the case of hexagonal lattice (Nelson and Halperin 1979), $\eta^*_{G_n}$ has no upper bound; since $\bar{K}_1^*$ can be arbitrarily close to zero, $\eta^*_{G_n}$ can be arbitrarily large.

3. Disclination-unbinding transition

3.1. Orientational order below and above T_m

Orientational order is reflected by the correlation function $C_\theta(\boldsymbol{r})$ defined in (1.6*a*). Below T_m, the average $\langle \psi(\boldsymbol{r})\psi^*(\boldsymbol{0})\rangle$ is evaluated over the total elastic energy H_E, defined in (2.1). Performing an average over H_E is equivalent to performing one over H_0 but with the replacement of all bare elastic constants by their renormalised values. This average is easily evaluated upon substituting the explicit form for $\psi(\boldsymbol{r})$ as defined in (1.6*b*) and we find that, for large $\boldsymbol{r}$,

$$\langle \psi(\boldsymbol{r})\psi^*(\boldsymbol{0})\rangle \sim \exp\left(-\frac{25k_B T\Lambda^2 K_{1R}(T)}{4\pi[\mu_R(T)K_{1R}(T) - K_{3R}^2(T)]}\right) \tag{3.1}$$

where Λ is an untraviolet cutoff. For $T < T_m$, stability requires that $K_{1R}(T) > 0$ and $\mu_R(T)K_{1R}(T) - K_{3R}^2(T) > 0$ (Levine *et al* 1985); thus

$$\langle \psi(\boldsymbol{r})\psi^*(\boldsymbol{0})\rangle \sim \text{constant} \tag{3.2}$$

indicating true long-range orientational order for $T < T_m$.

For temperatures above T_m, the behaviour of $\langle \psi(\boldsymbol{r})\psi^*(\boldsymbol{0})\rangle$ is determined by the effect of a gas of unbound dislocations on orientational fluctuations. If any residual orientational order persists, one would expect the energy associated with its fluctuations to be of the form (Nelson and Halperin 1979)

$$H_\theta = \tfrac{1}{2}K(T) \int d^2r |\bar{\nabla}\theta(\boldsymbol{r})|^2. \tag{3.3}$$

If we consider only the long-wavelength fluctuations of $\theta(\boldsymbol{r})$ then

$$k_B T/K = \lim_{q \to 0} (q^2/\Omega)\langle \hat{\theta}(\boldsymbol{q})\hat{\theta}(-\boldsymbol{q})\rangle \tag{3.4}$$

where $\hat{\theta}(\boldsymbol{q})$ is the Fourier transform of the bond-angle field $\theta(\boldsymbol{r})$ defined in (1.12b). Any smooth displacement fields will not contribute to the average in (3.4); the rotations induced by isolated dislocations, however, will. In our earlier work (De and Pelcovits 1987a) we have presented the displacement fields due to a single dislocations at the origin with Burgers' vector $\tilde{b}=(b_x, b_y, d_x, d_y)$. Calculating $\theta(\boldsymbol{r})$ from these displacement fields, we find the bond-angle field $\theta(\boldsymbol{r})$ due to a single dislocation at the origin. We can trivially generalise this to find the rotation field due to an arbitrary distribution of dislocations; the Fourier transform of the field is

$$\hat{\theta}(\boldsymbol{q}) = -\frac{\mathrm{i}\boldsymbol{q}\cdot\hat{\boldsymbol{b}}(\boldsymbol{q})}{q^2}+\frac{\mathrm{i}K_3K_1}{2(\mu K_1-K_3^2)}\left(\frac{q_x(q_x^2-3q_y^2)}{q^4}\hat{d}_x(\boldsymbol{q})+\frac{q_y(3q_x^2-q_y^2)}{q^4}\hat{d}_y(\boldsymbol{q})\right) \tag{3.5}$$

where $(\hat{b}_x, \hat{b}_y, \hat{d}_x, \hat{d}_y)$ is the Fourier transform of the four-dimension Burgers' vector field $\tilde{b}(\boldsymbol{r})=(\boldsymbol{b}(\boldsymbol{r})\oplus\boldsymbol{d}(\boldsymbol{r}))$. The two two-component fields $\boldsymbol{b}$ and $\boldsymbol{d}$ are not independent quantities (Levine *et al* 1985). For a given $\boldsymbol{b}$, we can parametrise $\boldsymbol{d}$ as

$$\boldsymbol{d}=\left(\frac{b_x(b_x^2-3b_y^2)}{b^2}, \frac{b_y(3b_x^2-b_y^2)}{b^2}\right). \tag{3.6}$$

If we use this relation in conjunction with (3.5), the expression in (3.4) expands as

$$\begin{aligned}\frac{k_\mathrm{B}T}{K}=\lim_{q\to 0}\left(\frac{1}{\Omega}\right)\Bigg[&\frac{q_iq_j}{q^2}\langle\hat{b}_i(\boldsymbol{q})\hat{b}_j(-\boldsymbol{q})\rangle+\frac{K_3^2K_1^2}{4(\mu K_1-K_3^2)^2}\\
&\times\left(\frac{q_x^2(q_x^2-3q_y^2)^2}{q^6}\left\langle\frac{\hat{b}_x(\boldsymbol{q})\hat{b}_x(-\boldsymbol{q})[\hat{b}_x^2(\boldsymbol{q})-3\hat{b}_y^2(\boldsymbol{q})][\hat{b}_x^2(-\boldsymbol{q})-3\hat{b}_y^2(-\boldsymbol{q})]}{\hat{b}^4}\right\rangle\right.\\
&+\frac{q_y^2(3q_x^2-q_y^2)^2}{q^6}\left\langle\frac{\hat{b}_y(\boldsymbol{q})\hat{b}_y(-\boldsymbol{q})[3\hat{b}_x^2(\boldsymbol{q})-\hat{b}_y^2(\boldsymbol{q})][3\hat{b}_x^2(-\boldsymbol{q})-\hat{b}_y^2(-\boldsymbol{q})]}{\hat{b}^4}\right\rangle\\
&+2\frac{q_xq_y(q_x^2-3q_y^2)(3q_x^2-q_y^2)}{q^6}\\
&\times\left.\left\langle\frac{\hat{b}_x(\boldsymbol{q})\hat{b}_y(-\boldsymbol{q})[\hat{b}_x^2(\boldsymbol{q})-3\hat{b}_y^2(\boldsymbol{q})][3\hat{b}_x^2(-\boldsymbol{q})-\hat{b}_y^2(-\boldsymbol{q})]}{\hat{b}^4}\right\rangle\right)\\
&+\frac{K_3K_1}{2(\mu K_1-K_3^2)}\left(\frac{q_x^2(q_x^2-3q_y^2)}{q^6}\left\langle\frac{\hat{b}_x(\boldsymbol{q})\hat{b}_x(-\boldsymbol{q})[\hat{b}_x^2(-\boldsymbol{q})-3\hat{b}_y^2(-\boldsymbol{q})]}{\hat{b}^2}\right\rangle\right.\\
&+\frac{q_y^2(3q_x^2-q_y^2)}{q^4}\left\langle\frac{\hat{b}_y(\boldsymbol{q})\hat{b}_y(-\boldsymbol{q})[3\hat{b}_x^2(-\boldsymbol{q})-\hat{b}_y^2(-\boldsymbol{q})]}{\hat{b}^2}\right\rangle\\
&+\frac{q_xq_y(q_x^2-3q_y^2)}{q^4}\left\langle\frac{\hat{b}_x(\boldsymbol{q})\hat{b}_y(-\boldsymbol{q})[\hat{b}_x^2(-\boldsymbol{q})-3\hat{b}_y^2(-\boldsymbol{q})]}{\hat{b}^4}\right\rangle\\
&\left.+\frac{q_xq_y(3q_x^2-q_y^2)}{q^4}\left\langle\frac{\hat{b}_x(\boldsymbol{q})\hat{b}_y(-\boldsymbol{q})[3\hat{b}_x^2(-\boldsymbol{q})-\hat{b}_y^2(-\boldsymbol{q})]}{\hat{b}^2}\right\rangle\right)\Bigg].\end{aligned} \tag{3.7a}$$

The averages in (3.7) are to be performed over the interaction energy of an arbitrary, not necessarily charge-neutral, distribution of dislocations. This energy is presented in De and Pelcovits (1987a). To perform the averages, we Fourier transform the interaction Hamiltonian and calculate the averages using Debye–Huckel theory, which amounts to treating $\hat{\boldsymbol{b}}(\boldsymbol{q})$ as a vector of continuous length (Nelson and Halperin 1979). For the sake of simplification, we note that our interest is in evaluating $k_\mathrm{B}T/K$ for

$T > T_m$ since we already know that, for $T < T_m$, long-range orientational order persists. For $T > T_m$, we substitute for the elastic constants in (3.7*a*) their renormalised values at T_m. Upon numerically integrating the renormalisation group equation (2.14) we have determined that $K_{1R}(T_m) = K_{2R}(T_m) = K_{3R}(T_m) = 0$. Thus, for $T > T_m$,

$$\frac{k_B T}{K} = \lim_{q \to 0} \frac{q_i q_j}{\Omega^2} \langle \hat{b}_i(\boldsymbol{q}) \hat{b}_j(\boldsymbol{q}) \rangle. \qquad (3.7b)$$

In performing the average, we likewise set $K_1 = K_2 = K_3 = 0$ into the expression for H_D, obtaining thus the simple results that, for $T > T_m$,

$$K = 2E_c a_0^2 \qquad (3.8)$$

where E_c is the core energy of a dislocation and is defined in De and Pelcovits (1987a). This establishes that orientational order does persists above T_m.

Having determined the value of K, it is straightforward to evaluate $\langle \psi(\boldsymbol{r}) \psi^*(\boldsymbol{0}) \rangle$ for $T > T_m$, where performing the average over H_θ in (3.3) gives

$$\langle \psi(\boldsymbol{r}) \psi^*(\boldsymbol{0}) \rangle \sim r^{-\eta_{10}} \qquad (3.9)$$

where

$$\eta_{10}(T) = \frac{50 k_B T}{\pi K(T)}. \qquad (3.10)$$

3.2. Second transition

The algebraic decay of the orientational order above T_m does not persist indefinitely. As the temperature is raised, screening due to increasing numbers of ±72° pairs of disclinations lead to a temperature T_i at which the pairs with the largest separation dissociate.

The total elastic energy in the presence of neutral pairs of disclinations can, as in the case of dislocations, be written as a sum:

$$H'_E = \tfrac{1}{2} K \int d^2 r |\nabla \phi|^2 + H'_D \qquad (3.11)$$

where we have decomposed the bond-angle field into a smoothly varying part ϕ and a multivalued part due to disclinations whose contribution to the elastic energy is H'_D.

Minimising the free energy density

$$f = \tfrac{1}{2} K \left[\left(\frac{\partial \theta}{\partial x} \right)^2 + \left(\frac{\partial \theta}{\partial y} \right)^2 \right] \qquad (3.12)$$

we find that, in the presence of disclinations, the bond-angle field satisfies

$$K_1 \nabla^2 \theta = 0 \qquad (3.13a)$$

for regions away from the core of a disclination while around the core, $\theta(\boldsymbol{r})$ satisfies (De and Pelcovits 1987b)

$$\oint d\theta(\boldsymbol{r}) = 2\pi s / 10 \qquad s = \pm 1, \pm 2, \ldots . \qquad (3.13b)$$

Solutions that satisfy (3.13) are easily obtained using the techniques outlined in De and Pelcovits (1987a) and we find that the energy due to such fields is

$$H'_{\mathrm{D}} = -\frac{\pi K}{100}\int \frac{\mathrm{d}^2 r}{a_0^2}\frac{\mathrm{d}^2 r'}{a_0^2} s(\boldsymbol{r})s(\boldsymbol{r})\ln\left|\frac{\boldsymbol{r}-\boldsymbol{r}}{a}\right| + E'_{\mathrm{c}}\int \mathrm{d}^2 r s^2(\boldsymbol{r}) \qquad (3.14)$$

where E'_{c} is the core energy of a disclination.

In De and Pelcovits (1988) we have presented the general expression for H'_{D} when $T < T_m$, i.e. in the presence of bound pairs of dislocations. It is worth noting that, in contrast to the latter energy, which increases as $R^2 \ln R$ where R is the size of the system, the energy in (3.14) has a weaker $\ln R$ dependence. This reduction in the interaction strength is due to the screening of disclinations by a gas of unbound dislocations.

The total energy H'_{E} in (3.11) is isomorphic to energy of spins in the XY model (Kosterlitz 1974). The results of that case are thus immediately reinterpreted as follows. The transition occurs at a temperature T_i such that

$$\eta_{10}(T_i) = \tfrac{1}{4} \qquad (3.15)$$

which implies that

$$\lim_{T\to T_i^-} K(T) = 100 k_{\mathrm{B}} T_i/\pi. \qquad (3.16)$$

For $T > T_i$, the orientational correlation function decays exponentially:

$$\langle \psi(\boldsymbol{r})\psi^*(\boldsymbol{0}) \sim \exp(-r/\xi_\theta) \qquad (3.17)$$

with the correlation length diverging as

$$\xi_\theta \sim \exp(\mathrm{c}|T - T_i|^{-1/2}) \qquad (3.18)$$

where c is a non-universal constant.

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