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**LETTER TO THE EDITOR**

# A field theory of dislocation mediated melting in two dimensions

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**Abstract.** It is shown that the theory of dislocation mediated melting in two dimensions is equivalent to a coupled vector sine-Gordon field theory. A systematic renormalisation group method for studying the transition is given. Recursion relations are obtained to second order in the dislocation activity for the case of melting on a periodic substrate.

In this Letter we point out that the theory of dislocation mediated melting in two dimensions (Kosterlitz and Thouless 1973, Halperin and Nelson 1978, Nelson and Halperin 1979, Young 1979) is equivalent to a coupled vector sine-Gordon field theory. Therefore, a systematic renormalisation group method for studying the melting transition can be developed along the lines of that given by Amit *et al* (1980) for the two-dimensional sine-Gordon theory (planar model, Coulomb gas). Recursion relations are obtained, to second order in the dislocation activity, for the general case of melting on a periodic substrate and found to agree with the results of Young (1979). It is relatively straightforward to generalise the calculations to higher order.

The energy of the dislocation system $H_D$ is given by continuum elasticity theory (Nabarro 1967). Defining $H_0 = -H_D/kT$, we have

$$H_0 = 2\pi \sum_{ij} [K_0^r (\boldsymbol{b}^i \cdot \boldsymbol{b}^j) \ln(r^{ij}/a_0) - K_0^\theta [(\boldsymbol{b}^i \cdot \boldsymbol{r}^{ij})(\boldsymbol{b}^j \cdot \boldsymbol{r}^{ij})/(r^{ij})^2 - \tfrac{1}{2}(\boldsymbol{b}^i \cdot \boldsymbol{b}^j)]] + \ln y_0 \sum_i (b^i)^2. \tag{1}$$

Here $\boldsymbol{r}^{ij} = \boldsymbol{r}^i - \boldsymbol{r}^j$ denotes the position of the $i$th dislocation with dimensionless Burgers vector $\boldsymbol{b}_i$, $\ln y_0$ is related to the core energy and $a_0$ is the lattice spacing. The dislocations are located on the sites of a dual lattice (which is hexagonal if the original lattice is triangular) and satisfy the neutrality condition $\Sigma_i \boldsymbol{b}_i = 0$. For an idealised 'floating' solid the coupling constants are equal, $K_0^r = K_0^\theta = K_0$ and

$$K_0 = \frac{1}{2\pi^2} \frac{\mu_0 B_0}{\mu_0 + B_0} \frac{a_0^2}{k_B T} \tag{2}$$

where $\mu_0$ and $B_0$ are the shear and bulk moduli in the absence of dislocations; however,

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in the general case when melting takes place on a substrate $K_0^r \neq K_0^\theta$ (Nelson and Halperin 1979). The Burgers vectors $\boldsymbol{b}^i$ lie on a Bravais lattice $\boldsymbol{b}^i = m^i\hat{\boldsymbol{e}}_1 + n^i\hat{\boldsymbol{e}}_2$, $m^i$ and $n^i$ are integers and $\hat{\boldsymbol{e}}_1$ and $\hat{\boldsymbol{e}}_2$ are unit vectors spanning the lattice. We will be concerned with the hexagonal lattice $\hat{\boldsymbol{e}}_1 \cdot \hat{\boldsymbol{e}}_2 = -\frac{1}{2}$. As only those dislocations with Burgers vectors of unit length are relevant, it will be convenient to introduce a triad of Bravais lattice vectors $\hat{\boldsymbol{e}}_1$, $\hat{\boldsymbol{e}}_2$ and $\hat{\boldsymbol{e}}_3$ which satisfy

$$\hat{\boldsymbol{e}}_i \cdot \hat{\boldsymbol{e}}_j = \tfrac{1}{2}(3\delta_{ij} - 1). \tag{3}$$

A standard choice is

$$\hat{\boldsymbol{e}}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \hat{\boldsymbol{e}}_2 = \begin{pmatrix} -1/2 \\ \sqrt{3}/2 \end{pmatrix} \qquad \hat{\boldsymbol{e}}_3 = \begin{pmatrix} -1/2 \\ -\sqrt{3}/2 \end{pmatrix}. \tag{4}$$

As we are concerned with large-distance behaviour, we may make a continuum approximation, allowing the vectors to be at any position rather than confined to lattice sites. The underlying lattice appears through the restriction that no two vectors may be closer than the lattice spacing $a_0$ which is necessary for stability. We therefore obtain a vector Coulomb gas with a hard-core repulsive interaction at short distances.

The Fourier transform of (1) may be written conveniently as

$$H_0 = \tfrac{1}{2}K \int \mathrm{d}^2q\, \boldsymbol{b}(\boldsymbol{q})\mathbf{G}(\boldsymbol{q})\boldsymbol{b}(-\boldsymbol{q}) + \ln y_0 \int \mathrm{d}^2q\, \boldsymbol{b}(\boldsymbol{q}) \cdot \boldsymbol{b}(-\boldsymbol{q}) \tag{5}$$

where the interaction between the vector charges has both transverse and longitudinal components,

$$\mathbf{G}(\boldsymbol{q}) = (q^2 + m_0^2)^{-1}(\mathbf{P}_\mathrm{T} + A_0\mathbf{P}_\mathrm{L}). \tag{6}$$

Here we have the projectors $\mathbf{P}_\mathrm{L} = \boldsymbol{qq}/q^2$, $\mathbf{P}_\mathrm{T} = \mathbf{I} - \boldsymbol{qq}/q^2$; the parameter $A_0 = K_\mathrm{L}/K_\mathrm{T}$ is the ratio of longitudinal to transverse couplings

$$K_\mathrm{T} = \tfrac{1}{2}(K_r + K_\theta) \tag{7}$$

$$K_\mathrm{L} = \tfrac{1}{2}(K_r - K_\theta) \tag{8}$$

$$8\pi^2 K_\mathrm{T} = K \tag{9}$$

and the mass $m_0$ has been introduced to regulate the infrared behaviour. In the case of the floating solid the interaction is purely transverse, $A_0 = 0$.

It is now straightforward to show that the vector Coulomb gas is equivalent to a coupled vector sine-Gordon field theory whose Lagrangian is

$$L = \tfrac{1}{2}\boldsymbol{\phi}\mathbf{G}^{-1}\boldsymbol{\phi} - \sum_{i=1}^{3} \frac{\alpha_0}{\beta_0^2 a_0^2}\cos(\beta_0 \hat{\boldsymbol{e}}_i \cdot \boldsymbol{\phi}). \tag{10}$$

Here $\beta_0^2 = K$, $\alpha_0$ is proportional to the dislocation activity, $y_0 = \alpha_0/2\beta_0^2$, and $\boldsymbol{\phi}$ is a two-component vector field. The free propagator of the theory, $\mathbf{G}$, which is just the interaction between dislocations (6) is given explicitly in coordinate space as

$$\mathbf{G}(\boldsymbol{x}) = [\mathbf{I} - (1 - A_0)\boldsymbol{\partial\partial}\partial/\partial m_0^2]K_0[m_0(x^2 + a_0^2)^{1/2}/2\pi] \tag{11}$$

which has the asymptotic form

$$\mathbf{G}(\boldsymbol{x}) = -\mathbf{I}\frac{(1 + A_0)}{8\pi}\ln[cm_0^2(x^2 + a_0^2)] + \frac{(1 - A_0)}{4\pi}\left(\frac{\boldsymbol{xx}}{x^2} - \frac{1}{2}\right) \tag{12}$$

for $m_0|x| \ll 1$. Here the lattice constant $a_0$ has been introduced as an ultraviolet regulator (Amit *et al* 1980) and $c = e^{2\gamma}/4$, where $\gamma$ is Euler's constant. To prove the equivalence it is sufficient to invoke a basic result of the theory of functional integration,

$$\int d[\phi] \exp\left(-\int \tfrac{1}{2}\boldsymbol{\phi}\mathbf{G}^{-1}\boldsymbol{\phi} + i\boldsymbol{J}\boldsymbol{\phi}\right) = \exp(-\tfrac{1}{2}\boldsymbol{J}\mathbf{G}\boldsymbol{J}). \tag{13}$$

Then, expanding the partition function

$$Z = \int d[\phi] \exp\left(-\int L d^2x\right) \tag{14}$$

as a power series in $\alpha_0$, the partition function of a vector Coulomb gas with reduced Hamiltonian given by (5) results.

The discussion of the melting transition now parallels the treatment of the planar model given by Amit *et al* (1980). The essence of the calculation is quite simple. It is shown that the vector sine-Gordon theory can be renormalised near $(\beta_0^2/16\pi)(1+A_0)$. The ultraviolet divergences of the one-particle irreducible two-point function $\boldsymbol{\Gamma}^{(2)}$ are located, expanded in a double series in $\alpha_0$ and $\delta_0 = (\beta_0^2/16\pi)(1+A_0)-1$, and then removed by appropriate renormalisation. Having the renormalisation constants, the renormalisation group flows are obtained by differentiating with respect to length scale.

The one-particle irreducible two-point function $\boldsymbol{\Gamma}^{(2)}$ can be written as

$$\boldsymbol{\Gamma}^{(2)} = \mathbf{G}^{-1} + \boldsymbol{\Sigma} \tag{15}$$

where $\boldsymbol{\Sigma}$ is the self-energy matrix. The diagrammatic rules that allow $\boldsymbol{\Sigma}$ to be represented to all orders in $\beta_0$ but to finite order in $a_0$ are similar to those of the sine-Gordon theory. The only change is that the vertices are labelled by an index $i$ indicating which $\cos(\beta\hat{\boldsymbol{e}}_i \cdot \boldsymbol{\phi})$ interaction occurs. The conventions are given in figure 1 and the contributions to $\boldsymbol{\Gamma}^{(2)}$ to order $\alpha_0^2$ are shown in figure 2. It is convenient to define a number of new functions:

$$I_{kl} = \beta_0^2 \hat{\boldsymbol{e}}_k \mathbf{G}(\boldsymbol{x}) \hat{\boldsymbol{e}}_l \tag{16}$$

$$B^k = \exp[-\tfrac{1}{2} I_{kk}(x^2 = 0)] \tag{17}$$

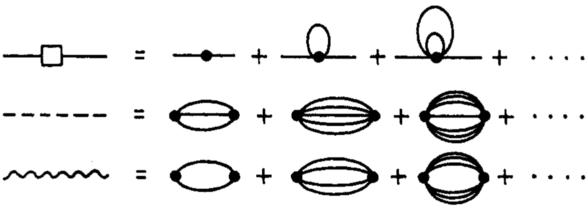

**Figure 1.** Diagrammatic convention for the renormalised $\alpha_0$ vertex, and the two propagators $(\cosh I(\boldsymbol{x}) - 1)$ and $(\sinh I(\boldsymbol{x}) - 1)$ that enter the theory.

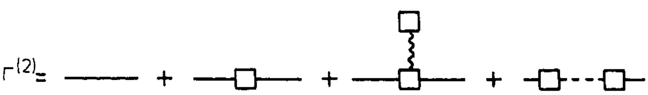


**Figure 2.** Diagrams contributing to the one-particle irreducible two-point function $\Gamma^{(2)}$ to order $\alpha_0^2$.

$$S_{kl} = \sinh I_{kl}(\boldsymbol{x}) \tag{18}$$

$$C_{kl} = \cosh I_{kl}(\boldsymbol{x}). \tag{19}$$

With these definitions and the notation of figures 1 and 2, we find $\boldsymbol{\Gamma}^{(2)}(p)$ to order $\alpha_0^2$ as

$$\boldsymbol{\Gamma}^{(2)}(p) = (p^2+m_0^2)\boldsymbol{I} + p^2\left(\mathbf{P}_\mathrm{T} + \frac{1}{A_0}\mathbf{P}_\mathrm{L}\right) + \frac{\alpha_0}{a^2}\sum_k B^k(\hat{\boldsymbol{e}}_k\hat{\boldsymbol{e}}_k)$$

$$+\frac{1}{\beta_0^2}\frac{\alpha_0^2}{a^2}\sum_{kl}[(\hat{\boldsymbol{e}}_k\hat{\boldsymbol{e}}_k)(C_{kl}(\boldsymbol{x})-1) - \mathrm{e}^{\mathrm{i}\boldsymbol{p}.\boldsymbol{x}}(\hat{\boldsymbol{e}}_k\hat{\boldsymbol{e}}_l)(S_{kl}(\boldsymbol{x})-I_{kl}(\boldsymbol{x}))] \tag{20}$$

where $(\hat{\boldsymbol{e}}_k\hat{\boldsymbol{e}}_k)$ is a matrix

$$(\hat{\boldsymbol{e}}_i\hat{\boldsymbol{e}}_j)_{kl} = (\hat{\boldsymbol{e}}_i)_k(\hat{\boldsymbol{e}}_j)_l. \tag{21}$$

The critical value of $\beta_0^2$ is determined by finding that value for which the renormalised coupling $\alpha_0 B^k/a_0^2$ is independent of $a_0$ (the condition that $\cos\beta(\boldsymbol{e}_i\,.\,\boldsymbol{\phi})$ is marginal). Equations (11) and (12) are combined to give $B^k$ as

$$B^k = [\exp(\beta_0^2/16\pi)](1+A_0)\ln(cm_0^2a^2) \tag{22}$$

which implies that the operator $\cos(\beta\hat{\boldsymbol{e}}_i\,.\,\boldsymbol{\phi})$ becomes marginal when

$$[(\beta_0^2)_c/16\pi](1+A_0) = 1. \tag{23}$$

Defining a new variable $\delta_0$ as

$$\delta_0 = (\beta_0^2/16\pi)(1+A_0)-1, \tag{24}$$

we may compute $\boldsymbol{\Sigma}$ to second order in a double expansion in $\alpha_0$ and $\delta_0$, focusing on the divergent terms.

At leading order in $\alpha_0$

$$\boldsymbol{\Sigma}^{(1)} = \tfrac{3}{2}\alpha_0(cm_0^2)[1+\delta_0\ln(cm^2a^2)+\ldots]\mathbf{I}. \tag{25}$$

It is only necessary to evaluate the divergent part of $\boldsymbol{\Sigma}^{(2)}$, and therefore it suffices to consider $\boldsymbol{\Sigma}^{(2)}(p^2=0)$ and $\partial^2\boldsymbol{\Sigma}^{(2)}/\partial\boldsymbol{p}\partial\boldsymbol{p}|_{p^2=0}$. Exploiting the invariance of the Lagrangian under $\mathrm{S}_3$, the group of permutations of the $\hat{\boldsymbol{e}}_i$'s, we may write the divergent part of $\boldsymbol{\Sigma}^{(2)}(p^2=0)$ as

$$\boldsymbol{\Sigma}^{(2)\mathrm{D}}(p^2=0) = \frac{3}{2\beta_0^2}\left(\frac{\alpha_0B^k}{a_0^2}\right)^2\mathbf{I}\int \mathrm{d}^2x\, C_{12}(\boldsymbol{x}). \tag{26}$$

The short-distance behaviour $(m_0|x|\ll 1)$ is given by

$$C_{12}(\boldsymbol{x}) \simeq \tfrac{1}{2}[cm^2(x^2+a^2)]^{-1}\exp\left(-\frac{\beta_0^2(1-A_0)}{4\pi}\frac{(\hat{\boldsymbol{e}}_1\,.\,\boldsymbol{x})(\hat{\boldsymbol{e}}_2\,.\,\boldsymbol{x})}{x^2+a_0^2}\right) \tag{27}$$

and therefore

$$\boldsymbol{\Sigma}^{(2)\mathrm{D}}(p^2=0) = -\alpha_0^2(cm^2)(3\pi/4\beta_0^2)\exp(\pi K^\theta/2)I_0(\pi K^\theta)\ln(cm_0^2a_0^2)\mathbf{I} \tag{28}$$

where $I_0$ is a modified Bessel function and

$$\pi K^\theta = \beta_0^2(1-A_0)/8\pi. \tag{29}$$

The other divergences of $\boldsymbol{\Sigma}^{(2)}$ are contained in

$$\tfrac{1}{2}p_kp_l\frac{\partial^2\boldsymbol{\Sigma}}{\partial p_k\partial p_l}\bigg|_{p^2=0} = \left(\frac{\alpha_0B^k}{a_0^2}\right)^2\frac{1}{2\beta_0^2}\int \mathrm{d}^2x(\boldsymbol{p}\,.\,\boldsymbol{x})^2\sum_{mn}(\hat{\boldsymbol{e}}_m\hat{\boldsymbol{e}}_n)[S_{mn}(\boldsymbol{x})-I_{mn}(\boldsymbol{x})]. \tag{30}$$

It is easy to see that the only divergences come from $S_{mn}(\boldsymbol{x})$; the result is

$$\tfrac{1}{2}p_k p_l \frac{\partial^2 \boldsymbol{\Sigma}}{\partial p_k \partial p_l}\bigg|_{p^2=0} = -\alpha_0^2 \frac{3\pi}{32\beta_0^2}\exp(\pi K^\theta)\ln(cm_0^2a_0^2)$$
$$\times\{[2I_0(\pi K^\theta)-I_1(\pi K^\theta)]p^2\mathbf{I}+2I_1(\pi K^\theta)\boldsymbol{pp}\}. \tag{31}$$

Combining (20), (25), (28) and (31), the expression for $\Gamma^{(2)}$ to second order in $\alpha_0$ and $\delta_0$ is

$$\begin{aligned}\boldsymbol{\Gamma}^{(2)}(p^2) = {} & m_0^2\mathbf{I}+p^2[\mathbf{P}_\mathrm{T}+(1/A_0)\mathbf{P}_\mathrm{L}]+\tfrac{3}{2}(\alpha_0cm^2)[1+\delta_0\ln(cm_0^2a_0^2)]\mathbf{I}\\ & -\alpha_0^2(cm^2)(3\pi/4\beta^2)\exp(\pi K^\theta/2)\ln(cm_0^2a_0^2)\mathbf{I}\\ & -\alpha_0^2(3\pi/32\beta_0^2)\exp(\pi K^\theta)\ln(cm_0^2a_0^2)\\ & \times[(2I_0(\pi K^\theta)-I_1(\pi K^\theta))\mathbf{P}_\mathrm{T}+(2I_0(\pi K^\theta)+I_1(\pi K^\theta))\mathbf{P}_\mathrm{L}].\end{aligned} \tag{32}$$

Renormalisation is carried out in the usual way; all divergences can be absorbed by three independent renormalisation constants $Z_\alpha$, $Z_\phi$ and $Z_A$. Renormalised quantities are defined by

$$\begin{aligned}\alpha_0 &= Z_\alpha\alpha\\ \beta_0^2 &= Z_\phi^{-1}\beta^2\\ m_0^2 &= Z_\phi^{-1}m^2\\ \phi^2 &= Z_\phi\phi_\mathrm{R}^2\\ A_0 &= Z^{-1}A\end{aligned} \tag{33}$$

and we require that the renormalised two-point vertex

$$\Gamma_\mathrm{R}^{(2)}(\boldsymbol{p},\alpha,\delta,m,\kappa) = Z_\phi\Gamma^{(2)}(\boldsymbol{p},\alpha_0,\delta_0,m_0^2,a) \tag{34}$$

is finite, order by order in the double expansion in $\alpha$ and $\delta$; $\kappa$ is a mass scale needed to define the renormalised theory. It is straightforward to find $Z_\alpha$, $Z_\phi$ and $Z_A$ by requiring that the coefficients of $m^2$, $p^2P_\mathrm{L}$ and $p^2P_\mathrm{T}$ be finite. We find

$$Z_\phi = 1+(3\pi/32\beta^2)[2I_0(\pi K^\theta)-I_1(\pi K^\theta)]\ln(k^2a^2) \tag{35}$$

$$Z_\phi Z_A = 1+(3\pi A/32\beta^2)[2I_0(\pi K^\theta)-I_1(\pi K^\theta)]\ln(k^2a^2) \tag{36}$$

$$Z_\alpha = 1-\delta\ln(k^2a^2)+(\alpha\pi/2\beta^2)I_0(\omega)\ln(k^2a^2). \tag{37}$$

The linear term in $\alpha$ arises because, unlike the planar model, the Lagrangian (10) is not invariant under $y\to -y$. Renormalisation group recursion relations are found by noting that the bare parameters cannot depend on the scale and differentiating with respect to length scale $L=\kappa^{-1}$:

$$\frac{\partial K_\mathrm{T}^{-1}}{\partial L} = \frac{\partial(\beta^2/8\pi^2)^{-1}}{\partial L} = (\beta^2/8\pi^2)^{-1}\frac{\partial\ln Z_\phi}{\partial L} \tag{38}$$

$$\frac{\partial K_\mathrm{L}^{-1}}{\partial L} = \frac{\partial(\beta^2A/8\pi^2)^{-1}}{\partial L} = (\beta^2A/8\pi^2)^{-1}\frac{\partial\ln Z_\phi Z_A}{\partial K} \tag{39}$$

$$\frac{\mathrm{d}y}{\mathrm{d}L} = \frac{\mathrm{d}(\alpha/2\beta^2)}{\mathrm{d}L} = \frac{1}{2}\alpha\beta^{-2}\frac{\partial\ln Z_\alpha Z_\phi}{\partial L}. \tag{40}$$

Using (35), (36) and (37) we find the recursion relations for the transverse and longitudinal couplings and dislocation activity

$$dK_L^{-1}/dL = 12\pi^3 y^2[I_0(\pi K^\theta) + \tfrac{1}{2}I_1(\pi K^\theta)]$$

$$dK_T^{-1}/dL = 12\pi^3 y^2[I_0(\pi K^\theta) - \tfrac{1}{2}I_1(\pi K^\theta)]$$

and

$$dy/dL = (2 - \pi K^r)y + 2\pi I_0(\pi K^\theta)y^2$$

are those given by Young (1979). Higher-order terms in the expansion are computable and will lead to universal corrections to the scaling form of correlation functions.

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