Dislocation Mediated Melting in Triangular Lattice

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The theory dislocation mediated melting is examined for triangular lattice in 2 dimensions. Recursion relations are extracted in terms of core energy of dislocation and their effective interactions. The divergence of correlation length close to critical temperature is calculated.

As stated in lecture notes in two dimensions, the Gold Stone modes destroys spontaneous order with broken continuous symmetry. Kosrelitz and Thouless [1] proposed a model for two dimensional melting. Based on their model the order in solid is destroyed by creation of dislocation pairs. As it was pointed out in the notes the close to critical temperature the correlation length does not diverge as power law which is a consequence of nonlinearity of recursion relations i.e.

$$\xi \propto \exp\left(\frac{c}{(T-T_c)^{\nu}}\right) \tag{1}$$

Where c is constant and ξ is the correltion length. T and T_c denote temperature and critical temperature, respectively. In this letter we will extract the recursion relations and consequently the exponent ν for triangular lattice. Halperin and Nelson [2] were the first one to calculate this exponent. However due to numerical error they incorrectly calculated $\nu = 0.44817$. Later, Young [3] calculated the the exponent properly $\nu = 0.36963$. In this work we follow the procedure portrayed in [4].

As it was shown in lecture notes, for triangular lattice in presence of dislocations, Kosrelitz and Thouless theory, $\beta\mathcal{H} = \beta\mathcal{H}_0 + \beta\mathcal{H}_1$ can be classified to two categories:

$$\begin{aligned}\beta\mathcal{H}_0 &= \frac{1}{2}\int d^2\mathbf{x}[2\mu\phi_{\alpha\beta}\phi_{\alpha\beta} + \lambda\phi_{\alpha\alpha}\phi_{\beta\beta}] \\ \beta\mathcal{H}_1 &= -\frac{K}{2\pi}\sum_{i<j}\left[\mathbf{b}_i.\mathbf{b}_j \log\left(\frac{|\mathbf{x}_i - \mathbf{x}_j|}{a}\right)\right. \\ &\quad \left. - \frac{(\mathbf{x}_i-\mathbf{x}_j).\mathbf{b}_i(\mathbf{x}_i-\mathbf{x}_j).\mathbf{b}_j}{|\mathbf{x}_i-\mathbf{x}_j|^2}\right] - \log y_0 \sum_i |\mathbf{b}_i|\end{aligned} \tag{2}$$

Here $\phi_{\alpha\beta}$ represents the smooth strain field. $\mathbf{b}_i$ denote the burger vectors. $\log y_0$ is related to core energy and a is lattice spacing, μ, and λ are lame constants, and $Ka^2 = 2\mu(\mu+\lambda)/(2\mu+\lambda)$. The dislocations are located on the sites of dual lattice and must satisfy the neutrality condition $\sum_i \mathbf{b}_i = 0$ and burger vectors are of unit length. For triangular lattice we consider the following unit vectors for burger vectors

$$\mathbf{e}_m = \left\{\begin{array}{c}\cos(2\pi m/3)\\ \sin(2\pi m/3)\end{array}\right\}, \quad m = 0, \cdots, 2. \tag{3}$$

which can be either be in positive or negative direction.

The approach here differs somewhat from the one presented in the lecture notes, instead of deriving the effective K, we derive the effective lame coefficients and extract K_{eff} as follows:

$$K_{eff}^{-1} = \frac{1}{2}\left(\frac{1}{\mu_{eff}} + \frac{1}{\mu_{eff}+\lambda_{eff}}\right) \tag{4}$$

In order to calculate the the effective lame constants, we have to calculate the the probability of dislocation pairs separated by R and with orientation θ, see Fig. (1-a) . However in order to calculate the recursion relations to the second order of y_0, we need to consider the pairs such as the one shown in Fig. (1-b). In such pairs two dislocation coalesce to one separated by r which is of the order of lattice spacing, and R determines the distance between the isolated dislocation and the center of mass of the coalesced ones. We note that each configuration of R and θ is consisted of three configurations based on the 3 basis vectors Eq. 3. Using Eq. 2 one can calculate the probability of such pairs

$$\begin{aligned}P_m = y_0^2\left(\frac{R}{a}\right)^{-K/2\pi}&\exp\left(\frac{K}{2\pi}\cos^2(\theta - m\frac{2\pi}{3})\right)\Bigg[1+ \\ 2y_0\int_0^{2\pi} d\phi &\exp\left(-\frac{K}{2\pi}\cos(\phi-\frac{\pi}{3})\cos(\phi+\frac{\pi}{3})\right) \\ \times\int_a^{ba}\frac{dr}{a}&\left(\frac{r}{a}\right)^{1-K/4\pi} + \mathcal{O}(y_0^2)\Bigg], \quad m = 0,1,2.\end{aligned} \tag{5}$$

which simplifies to

$$\begin{aligned}P_m = y_0^2\left(\frac{R}{a}\right)^{-K/2\pi}&\exp\left(\frac{K}{2\pi}\cos^2(\theta - m\frac{2\pi}{3})\right)\Bigg[1+ \\ 4\pi e^{K/8\pi} y_0 I_0(K/4\pi)&\int_a^{ba}\frac{dr}{a}\left(\frac{r}{a}\right)^{1-K/4\pi} + \mathcal{O}(y_0^2)\Bigg] \\ m = 0,1,2.&\end{aligned} \tag{6}$$

Please note that in the second term we have considered the rescaling of b. Using the method presented in [4] one can arrive at

$$C^{-1}_{eff,ijkl} = C^{-1}_{ijkl} + \frac{y_0^2}{4}\sum_{p=0}^{2}(\mathbf{e}_{p,i}\epsilon_{js} + \mathbf{e}_{p,j}\epsilon_{is}) \quad (7)$$

$$(\mathbf{e}_{p,k}\epsilon_{lt} + \mathbf{e}_{p,l}\epsilon_{kt})\int_0^{2\pi}\int_a^{\infty}\frac{dR}{a}\frac{R}{a}\frac{R_sR_t}{a^2}P_p \quad (8)$$

where

$$\epsilon = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}. \quad (9)$$

from Eq. 7 we extract the Lame coefficients and insert into Eq. 4 to derive the effective interaction

$$K^{-1}_{eff} = K^{-1} + \frac{3\pi}{2}e^{K/4\pi}y_0^2\left[2I_0\left(\frac{K}{4\pi}\right) - I_1\left(\frac{K}{4\pi}\right)\right]$$
$$\int_a^{\infty}\frac{dR}{a}\left(\frac{R}{a}\right)^{3-K/2\pi}\Bigg[1 + 4\pi e^{K/8\pi}y_0 I_0(K/4\pi)$$
$$\times\int_a^{ba}\frac{dr}{a}\left(\frac{r}{a}\right)^{1-K/4\pi} + \mathcal{O}(y_0^2)\Bigg] \quad (10)$$

by varying the cutoff a to ba, and assuming $b \approx 1 + l$

$$\begin{cases} \frac{dK^{-1}}{dl} = \frac{3}{2}\pi y_0^2 e^{K/4\pi}\left[2I_0\left(\frac{K}{4\pi}\right) - I_1\left(\frac{K}{4\pi}\right)\right] \\ \frac{dy_0}{dl} = \left(2 - \frac{K}{4\pi}\right)y_0 + 2\pi y_0^2 e^{K/8\pi}I_0\left(\frac{K}{4\pi}\right) \end{cases} \quad (11)$$

using the transformation $x = 8\pi K^{-1} - 1$ we arrive at recursion relation

$$\begin{cases} \frac{dx}{dl} = 12\pi^2 A y_0^2 \\ \frac{dy_0}{dl} = 2xy_0 + 2\pi B y_0^2 \end{cases} \quad (12)$$

where

$$A = e^2\left[2I_0(2) - I_1(2)\right], \quad B = eI_0(2). \quad (13)$$

The two solution that passes through the fixed point ($x = y_0 = 0$) are straight lines (separatrices) with slope m can be calculated by solving $y_0 = mx$, we arrive at

$$m_\pm = (1/12\pi A)(B \pm \sqrt{B^2 + 24A}) \quad (14)$$

We are more interested in the negative slope pertaining to below melting temperature, we can find the solutions calculated by $y_0 = mx$

$$x = \frac{-1}{12\pi^2 A m_-^2}\frac{1}{l + l_0}, \quad y = \frac{-m_-}{12\pi^2 A m_-^2}\frac{1}{l + l_0}, \quad (15)$$

we now assume that T is below T_c and $t = (T - T_c)/T_c \ll 1$

$$y_0(l) = m_- x(l) + D(l) \quad (16)$$

$$\frac{dD}{dl} = -2xD - \frac{2}{m}D^2 \quad (17)$$

replacing $x(l)$ from Eq. 15 in above equation to the first order of $D(l)$

$$D(l) = D_0(l + l_0)^{1/6\pi^2 m_-^2 A} \quad (18)$$

We can explore the nature of divergence close to critical temperature by considering $D_0 \approx |t|$, Eq. 16 is valid up to a length l^*. This length can be calculated when $x(l)$ is of order of $D(l)$

$$|t|(l^* + l_0)^{1/6\pi^2 m_-^2 A} \sim \frac{1}{l^* + l_0} \quad (19)$$

and resulting in

$$l^* \sim |t|^{-\nu} \quad \nu = \frac{6\pi^2 m_-^2 A}{1 + 6\pi^2 m_-^2 A} = 0.36963, \quad (20)$$

Now we are ready to explore the divergence of correlation length

$$\xi \approx a e^{l^*} \propto e^{c/|t|^{\nu}} \quad (21)$$

where c is a constant.

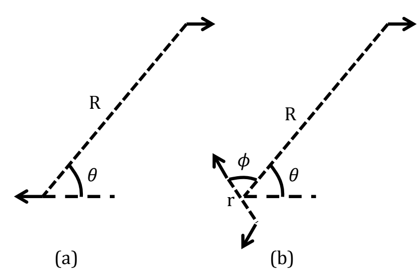

FIG. 1. (a) Schematic of a dislocation pair created in a triangular lattice (b) dislocation pair created by a pair of coalesced dislocation and an isolated one

[1] J. M. Kosterlitz and D. J. Thouless. Ordering, metastability and phase transitions in two-dimensional systems. *Journal of Physics C: Solid State Physics*, 6(7):1181, April 1973.

[2] B. I. Halperin and David R. Nelson. Theory of two-dimensional melting. *Physical Review Letters*, 41(2):121–124, July 1978.

[3] A. P. Young. Melting and the vector coulomb gas in two dimensions. *Physical Review B*, 19(4):1855–1866, February 1979.

[4] David R. Nelson and B. I. Halperin. Dislocation-mediated melting in two dimensions. *Physical Review B*, 19(5):2457–2484, March 1979.