1 Lecture 11: 2D melting mediated by topological defects. Instantons in nonlinear sigma model.

Recall the standard picture of melting (Lecture 3), describing transition from uniform liquid state to spatially modulated crystal state

$$\rho(\mathbf{x}) = \sum_{\mathbf{k}\in L} e^{i\mathbf{k}\cdot\mathbf{x}} \rho_{\mathbf{k}} \tag{1}$$

by density harmonic amplitude order parameter $\rho_{\mathbf{k}}$. Here the wavevectors $\mathbf{k}$ define density waves with the periodicity of a crystal. The Landau free energy, expanded in powers of $\rho_{\mathbf{k}}$, admits cubic invariants, which explains why melting is always a first order transition.

However, a completely different scenario of melting exists in 2D systems, built on an analogy between vortices in the XY model and dislocations in a 2D crystal. Dislocations (see Figure) are topological defects in crystals. Indeed, although crystal structure is perfect and ordered away from a dislocation center, after going around a dislocation and counting crystal rows one can detect dislocation at an arbitrarily large distance away from it.

A dislocation, if present, cannot be eliminated by any rearrangement of atoms in a crystal. To remove dislocation from a crystal, one has to merge it with a dislocation of opposite sign, so that the two dislocations annihilate each other. (In a finite system, one can also remove a dislocation by moving it to the boundary.) Because of that, dislocations are called *topological defects*, in contrast to other defects (e.g. vacancies, interstitials, etc. which change crystal properties only locally, and are "invisible" from far away.

The deformation of crystal lattice around a dislocation satisfies

$$\oint du_i(\mathbf{x}) = \oint \frac{\partial u_i}{\partial x_k} dx_k = -b_i \tag{2}$$

where $\mathbf{b}$ is the so-called Burgers vector of the dislocation. For simple dislocations this vector is one of the crystal lattice basis vectors. Mathematically, a dislocation with $\mathbf{b}$ being any lattice vector can be constructed, but since the dislocation energy scales with $\mathbf{b}^2$ (see below), usually only short length Burgers vectors are realized.

Topological nature of dislocations is best illustrated by the fusion rule: two dislocations with Burgers vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ from far away look like one dislocation with Burgers vector $\mathbf{b} = \mathbf{b}_1 + \mathbf{b}_2$. In particular, two dislocations with opposite vectors $\mathbf{b}$ and $-\mathbf{b}$ together are equivalent to a dislocation free crystal. A useful exercise is to verify that such a pair of a dislocation and an anti-dislocation can be eliminated by moving dislocations to each other and merging them together.

To find the energy of a dislocation, we use the expression for the elastic energy in terms of the deformation tensor $u_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i)$, and rewrite it in terms of the displacement field:

$$E(u) = \int \left(\frac{\lambda}{2} u_{ii}^2 + \mu u_{ij}^2 \right) d^2x = \int \left(\frac{1}{2}(\lambda+\mu)(\partial u_i/\partial x_i)^2 + \frac{1}{2}\mu(\partial u_i/\partial x_j)^2 \right) d^2x \qquad (3)$$

with Lame constants λ, μ. Displacement field distribution around a dislocation is anisotropic, it has both angular and radial dependence. Thus it would be impossible to guess its form, as we did for vortices in the XY model. Instead, we shall use a trick and calculate the dislocation interaction energy directly, using Fourier representation.

We define a quantity $w_{ij} = \partial u_i/\partial x_j$. Using this definition, the energy of a system of dislocations at $\mathbf{x} = \mathbf{x}_n$ with Burgers vectors $\mathbf{b}_n$ can be written as

$$E = \int \left(\frac{1}{2}(\lambda+\mu) w_{ii}^2 + \frac{1}{2}\mu w_{ij}^2 + \phi_i(\mathbf{x}) \left(\epsilon_{jj'} \partial_j w_{j'i} - b_i(\mathbf{x}) \right) \right) d^2x \qquad (4)$$

with 2×2 antisymmetric tensor $\epsilon_{jj'}$ and

$$\mathbf{b}(\mathbf{x}) = \sum_n \mathbf{b}_n \, \delta(\mathbf{x} - \mathbf{x}_n) \qquad (5)$$

Here $\phi_i(\mathbf{x})$ is a Lagrange multiplier field enforcing the relation of distortion with Burgers vectors. We have $\partial_j w_{j'i} - \partial_{j'} w_{ji} = 0$ away from dislocation cores, where the displacement field u_i is single-valued.

To minimize energy in w_{ij}, we first move the derivative on $\phi_i(\mathbf{x})$, integrating by parts. We minimize

$$\frac{1}{2} u_{ij} w_{ij}^2 - g_{ij} w_{ij} \,, \quad g_{ij} = \epsilon_{j'j} \partial_{j'} \phi_i \,, \quad u_{ij} = \begin{cases} \lambda + 2\mu & i = j \\ \mu & i \neq j \end{cases} \qquad (6)$$

which gives

$$\int \left(-\frac{1}{2\mu} g_{ij}^2(\mathbf{x}) + \left(\frac{1}{2\mu} - \frac{1}{2(\lambda+2\mu)} \right) g_{ii}^2(\mathbf{x}) - \phi_i(\mathbf{x}) b_i(\mathbf{x}) \right) d^2x \qquad (7)$$

To minimize in ϕ, we rewrite this expression in Fourier components,

$$\sum_q \left(-\frac{1}{2\mu} |q'_i \phi_j(q)|^2 + \frac{\lambda+\mu}{2\mu(\lambda+2\mu)} |q'_i \phi_i(q)|^2 - \phi_i(q) b_i(-q) \right) \qquad (8)$$

with $q'_i = \epsilon_{ij} q_j$, the vector $\mathbf{q}$ rotated by $\pi/2$. Minimizing this expression in $\phi_i(q)$, obtain

$$E = \sum_q \frac{1}{2} b_i(-q) K_{ij} b_j(-q) \,, \quad K_{ij}^{-1} = \frac{1}{\mu} (\mathbf{q}')^2 \delta_{ij} + \frac{\lambda+\mu}{\mu(\lambda+2\mu)} q'_i q'_j \qquad (9)$$

Fourier transforming back to real space, we have

$$E = \frac{1}{2} \iint b_i(\mathbf{x}) K_{ij}(\mathbf{x}-\mathbf{x}') b_j(\mathbf{x}') \,, \quad K_{ij}(\mathbf{y}) = \int \left(\frac{1}{\mu} (\mathbf{q}')^2 \delta_{ij} - \frac{\lambda+\mu}{\mu(\lambda+2\mu)} q'_i q'_j \right)^{-1} e^{i\mathbf{q}\cdot\mathbf{y}} \frac{d^2q}{(2\pi)^2} \qquad (10)$$

Finally, after evaluating the integral for $K_{ij}(\mathbf{y})$ and inserting the dislocation density in the form (5), obtain

$$E = -\frac{1}{8\pi}\sum_{\mathbf{x}\neq\mathbf{x}'}\left(K_1\mathbf{b}(\mathbf{x})\cdot\mathbf{b}(\mathbf{x}')\ln(|\mathbf{x}-\mathbf{x}'|/a) - K_2\frac{\mathbf{b}(\mathbf{x})\cdot(\mathbf{x}-\mathbf{x}')\mathbf{b}(\mathbf{x}')\cdot(\mathbf{x}-\mathbf{x}')}{|\mathbf{x}-\mathbf{x}'|^2}\right) \quad (11)$$

with

$$K_{1,2} \equiv K = \frac{4\mu(\mu+\lambda)}{\lambda+2\mu} \quad (12)$$

The dominant interaction is logarithmic at large distances.

Possible phases of the system of interacting dislocations can be discussed in the same way as in our analysis of Coulomb gas in the XY problem. If $\beta K/8\pi$ is less than 2, the entropic effects favor unbound dislocations. On the other hand, for $\beta K/8\pi$ larger than 2, the strong interaction leads to dislocations binding in topologically neutral pairs, and freezing at macroscopic distances.

From symmetry viewpoint, the dislocation-free state at $\beta K > 8\pi$ is a periodic crystal with translational order. The high temperature state, $\beta K < 8\pi$, due to a finite density of dislocations does not possess long range translational order. In its symmetry, however, this state is different from liquid, since it has a six-fold rotational symmetry. (A true liquid is fully isotropic, its rotational symmetry group is $O(2)$.) Such order is called a *hexatic state*. It is similar in it properties to liquid crystal order in a nematic state, in that there is a preferred direction at every point of the system. The difference is that there are three equivalent directions at each point of a hexatic phase, at $\pi/3$ angle to each other, while there is only one direction in nematic.

Renormalization group at the dislocation melting transition point $\beta K = 16\pi$ can be constructed as in the XY model (Halperin and Nelson, 1979). The crucial difference compared to the XY model is that there are three equivalent Burgers vector directions (six if signs are distinguished). As in the the XY problem, it is sufficient to take into account only the shortest vectors, which are the triangular lattice basis vectors

$$\pm\mathbf{e}_1, \quad \pm\mathbf{e}_2, \quad \pm\mathbf{e}_3, \quad (13)$$

with $\mathbf{e}_1+\mathbf{e}_2+\mathbf{e}_3 = 0$. Fusion rules for these dislocations are less trivial than for the vortices in the XY problem. We still have that a dislocation pair with equal and opposite Burgers vectors is topologically neutral at large distances. In addition, however, two dislocations with, for example, vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ collectively form a pair with a net Burgers vector $\mathbf{e}_1 + \mathbf{e}_2 = -\mathbf{e}_3$. Because of that, when we sum over dislocation configurations at short distances in order to obtain effective interaction at larger distances, dislocation fusion contributes an additional term to the Kosterlitz-Thouless RG equations:

$$\frac{dK^{-1}(l)}{dl} = c_1 y^2(l)\,, \quad \frac{dy(l)}{dl} = (2 - K(l)/8\pi)y(l) + c_2 y^2(l) \quad (14)$$

with $y(l)$ the dislocation statistical weight, $l = \ln\Lambda/\Lambda'$ the RG "time," and $c_{1,2}$ positive constants describing interaction screening by neutral pairs, and fusion of non-neutral pairs. (Here we used dimensionless rigidity K scaled by temperature.)

The new term changes the RG flow. This affects the temperature dependence of the correlation length

$$\xi(T) \propto \exp(b/|T - T_c|^\nu) , \quad \nu = 0.3696... \tag{15}$$

instead of $\nu = 1/2$ in the XY model. The Lame constants μ and λ drop to zero at the transition, so that the combination $\mu(\lambda + \mu)/(\lambda + 2\mu)$ has a universal jump of $8\pi T_c/a^2$, where a is the lattice constant (Burgers vector length).

As the temperature is increased further, the hexatic state should disappear giving rise to a true liquid. This transition can also be mediated by topological defects, *disclinations.* A disclination is a singularity of an orientational order parameter, such that the local crystal axis direction rotates by a multiple of $\pi/3$ going around the disclination center. Then theory of disclination melting is very similar to that developed for the XY problem. Thus in this *defect mediated* melting scenario, instead of one first order transition predicted by Landau theory, we have two subsequent second order transitions, each being a topological transition of Kosterlitz-Thouless kind.

The scenario of melting induced by topological defects is very appealing. In real systems, however, it may or may not be realized depending on relative importance of the fluctuations caused by topological defects and other thermal fluctuations that can cause crystal melting via a first order transition. A number of systems, in which melting is suspected to be topological, have been studied, with no conclusive results so far.

1.1 Instantons

to be discussed after Spring break, on March 31 (?)