Topological aspect of disclinations in two-dimensional melting

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By using topological current theory, we study the inner topological structure of disclinations during the melting of two-dimensional systems. From two-dimensional elasticity theory, it is found topological currents for topological defects in homogeneous equation. The evolution of disclinations is studied, and the branch conditions for generating, annihilating, crossing, splitting and merging of disclinations are given.

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Topological defects, which are a necessary consequence of broken continuous symmetry, play an important role in two-dimensional phase transition. In 1970’s, Kosterlitz and Thouless construct a detailed and complete theory of superfluidity on two-dimensions[1]. They indicate vortices pair unbinding will lead to a second-order transition in superfluid films. Later, a microscopic scenario of 2D melting has been posited in the form of the Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) theory[2,3,4]. The KTHNY theory predicts a new phase, the so-called hexatic phase, that exists between the solid and liquid phases in 2D melting[5].

In two-dimensional colloidal systems, topological defects have been studied in experiments and computer simulations. A serial experiments were performed to calculate dislocations and disclinations dynamic of two-dimensional colloidal systems, and dissociation of dislocations and disclinations were observed[6,7,8,11]. During the years, a large number of computer simulations indicated that exist a two-stage melting as prescribed by KTHNY theory, however, results are still controversial[12,13,14,15]. Although the KTHNY theory is currently preferred, a different theoretical approach, evoking grain-boundary-induced melting, was a first-order transition suggested by Chui[16]. One may note that the condensation of geometrical defects is also a first-order transition[17,18]. Our previous work found that exist a hexatic-isotropic liquid phase coexistence during the melting of soft Yukawa systems[19,20]. By Voronoï polygons analysis, the behavior of point defects in the coexistence is very complicated. The evolution of topological defects during the melting of two-dimensional system still a open question.

Recently, a topological field theory for topological defects developed by Duan et al[21], By using Duan’s topological current theory, the inner topological structure and bifurcation of topological defects, such as disclination and dislocation in liquid crystal and solid, were studied. In KT phase transition, there also exists an elementary vortex topological current constructed by the superfluid order parameter[22]. By using the topological current theory, we can give the the branch conditions for generating, annihilating, crossing, splitting and merging of topological defects.

In this paper, we will discuss the topological quantization and bifurcation of topological defects in two-dimensional crystals. This work is based on the so-called Duan’s topological current theory. The organization of this paper is as follows. We describe the elasticity theory. Using Duan’s topological current theory, we discussed the topological structure of disclination in two-dimensional crystals. In the last section, we summarize our results.

In continuum elasticity theory, the elastic Hamiltonian in two-dimensional triangular solid is given by[22]

\[
F = \frac{1}{2} \int d^2r (2\mu u^2_{ij} + \lambda u^2_{kk}),
\]

where \(\lambda\) and \(\mu\) are the two-dimensional Lamé coefficients. The strain tensor is

\[
u_{ij}(r) = \frac{1}{2} \left[ \frac{\partial u_i(r)}{\partial r_j} + \frac{\partial u_j(r)}{\partial r_i} \right]
\]

A deformation is represented by a displacement vector field \(\mathbf{u}(r) = (u_x, u_y)\), which maps the point \(\mathbf{r} = (x, y)\) to \(\mathbf{r} + \mathbf{u}\). If there are no defects, the deformation is a single-valued mapping of the plane onto itself. But \(\mathbf{u}\) becomes a multi-valued function when there is a dislocation. A single dislocation corresponds to an extra half lattice plane, which characterized by a Burger’s vector \(\mathbf{b}\). Another type of defect in two-dimension crystal is disclination, which is defined in terms of the bond angle field \(\theta\). \(\theta(x)\) is the angle between local lattice bonds and a reference axis.

If we minimize \(F\) with respect to variations in \(\mathbf{u}\), we obtain the equation

\[
\partial_i\sigma_{ij} = 0,
\]

where the stress tensor \(\sigma_{ij}\) is defined by

\[
\sigma_{ij} = 2\mu u_{ij} + \lambda u_{kk}\delta_{ij},
\]

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Because $\sigma_{ij}$ is symmetric, it can be written as

$$\sigma_{ij} = \epsilon_{ik}\epsilon_{jl} \nabla_k \nabla_l \chi, \quad (5)$$

The function $\chi$ is called the Airy stress function. Although any choice for $\chi$ yields a stress tensor that satisfies Eq. (3), the choice cannot be arbitrary. The strain $u_{ij}$ is related to the stress is

$$u_{ij} = \frac{1}{2\mu} \sigma_{ij} - \frac{\lambda}{4(\mu + \lambda)} \delta_{ij} \sigma_{kk}$$

$$= \frac{1}{\mu} + \frac{\delta_{ij}}{\mu} \epsilon_{ik}\epsilon_{jl} \nabla_k \nabla_l \chi - \frac{\sigma_0}{\mu} \nabla^2 \delta_{ij} \quad (6)$$

where $Y = 4\mu(\mu + \lambda)/(2\mu + \lambda)$ is the two-dimensional Young’s modulus and $\sigma_0 = \lambda/(2\mu + \lambda)$ the two-dimensional Poisson ratio. Applying $\epsilon_{ik}\epsilon_{jl} \nabla_k \nabla_l$ to both sides of this equation, we find

$$\nabla^4 \chi = \frac{1}{\mu} \epsilon_{ik}\epsilon_{jl} \nabla_k \nabla_l \left( \partial_i u_j + \partial_j u_i \right)$$

$$= \frac{1}{\mu} \epsilon_{ik}\epsilon_{jl} \nabla_k \nabla_l \left( \partial_i u_j - \partial_j u_i + \partial_i u_j \right)$$

$$= \epsilon_{ik}\epsilon_{jl} \nabla_k \nabla_l \chi + 2 \epsilon_{ik}\epsilon_{jl} \nabla_k \nabla_l \chi$$

$$(7)$$

The defects associated with the continuum elastic theory of a solid are dislocations and disclinations. Dislocations and disclinations can be introduced into the theory in a way similar to the discussion of superfluid vortices\[1\]. In the following we consider only the triangular lattice in a way similar to the discussion of superfluid vortices. Disclinations are characterized by a topological charge, which measures the bonds orientation. It is convenient to define an order parameter for bond orientations, which are symmetric and favored by Nature.

Disclinations, which are characterized by a topological charge, have a much higher energy than dislocations. They are defined in terms of the bond angle field $\theta(r)$, which measures the bonds orientation. It is convenient to define an order parameter for bond orientations, which for the triangular lattice is $\psi(r) = \psi_0 e^{i\theta(r)}$. However, the bond angle field is undefined at the disclination cores, i.e., the zero points of the order parameter. We rewrite the bond angle field $\theta(r)$ as

$$\phi_0^a(x, y) = 0, \quad \phi_0^2(x, y) = 0. \quad (9)$$

Suppose there is a defect located at $z_i$, the topological charge of the defect is defined by the Gauss map $\Psi$, i.e.,

$$W(\phi_0, z_i) = \frac{1}{2\pi} \oint_{\partial S_i} \epsilon_{ab} n^a \epsilon_{b} \quad (10)$$

Using the Stokes’ theorem in the exterior differential form, one can deduce that

$$W(\phi_0, z_i) = \frac{1}{2\pi} \oint_{\partial S_i} \epsilon_{ab} \epsilon_{ij} \partial_i \phi_a \partial_j \phi_b \quad (11)$$

We can deduce a topological current of disclinations in two-dimensional crystal,

$$j^k_{\text{disc}} = \frac{1}{6} \epsilon_{ijk} \epsilon_{ab} \partial_i \phi_a^b \delta_j \phi_b^c = \delta^2(\phi_0) J^k \left( \frac{\phi_0}{x} \right) \quad (12)$$

It is easy to see that this topological current is identically conserved, i.e.,

$$\partial_j j^k = 0. \quad (14)$$

According to the implicit function theorem, if Jacobian determinant

$$J^0 \left( \frac{\phi_0}{x} \right) = J \left( \frac{\phi_0}{x} \right) \neq 0, \quad (15)$$

the solutions of Eq. (9) can be generally expressed as

$$x = x(t), \quad y = y(t), \quad l = 1, 2, ..., N, \quad (16)$$

which represent N zero points $z_i(t)$ for the line of N disclinations $D_t$ in space-time.

With the $\delta$-function theory, $\delta^2(\phi)$ can be expanded as

$$\delta^2(\phi_0) = \sum_{i=1}^{N} \frac{\beta_i}{|J(\phi_0/x)|_{z_i}} \delta^2(\phi - \phi_0) \quad (17)$$

where the positive integer $\beta_i$ is called the Hopf index of the zero $z_i$ once, the vector field $\phi_0$ covers the corresponding region for $\beta_i$ times. Using the implicit function theorem and the definition of

![FIG. 1: Disclination in triangular lattices. A $-\pi/3$ disclination with its sevenfold coordinated site in the center (left). A $\pi/3$ disclination with its fivefold coordinated site (right).](image)
vector Jacobians, we can get the velocity of the l-th defect,

\[ \vec{v}_l = \frac{d\vec{z}_l}{dt} = \frac{\vec{J}(\phi_6/x)}{J(\phi_6/x)} \cdot \vec{z}_l \]

Then the spatial and temporal components of the defect current $j_u$, can be written as the form of the current and the density of the system of N classical points particles with topological charge $W_l = \beta_l \eta_l$ moving in the (2+1)-dimensional space-time,

\[ \vec{j} = \sum_{l=1}^{N} \beta_l \eta_l \vec{v}_l \delta^2(\vec{r} - \vec{z}_l(t)) \]  

(19)

\[ \rho = \sum_{l=1}^{N} \beta_l \eta_l \delta^2(\vec{r} - \vec{z}_l(t)) \]  

(20)

where $\eta_l$ is Brouwer degree,

\[ \eta_l = \frac{J(\phi_6/x)}{J(\phi_6/x)} \bigg|_{\vec{z}_l} = \pm 1 \]  

(21)

For disclinations, using Duan’s topological current theory the homogeneous equation can write as

\[ \frac{1}{Y} \nabla^2 \chi = \frac{2\pi}{6} \delta^2(\phi_6) J(\phi_6/x) \]  

(22)

Similar results get by Nelson in the KTHNY theory. In our theory, the topological charge of a disclination $D_l$ is

\[ Q_l = \int_{\Sigma_l} \epsilon_{ij} \partial_i n^a_6 \partial_j n^b_6 d^2x \]

(23)

where $W_l$ is the winding number of $\Psi$ around $D_l$, the above expression reveals distinctly that the topological charge of disclination is not only the winding number, but also expressed by the Hopf indices and Brouwer degrees. The topological inner structure showed in Eq. (23) is more essential than that in Eq. (7), this is the advantage of our topological description of the disclination.

It is clearly seen that Eq. (19) shows the movement of two-dimension crystal topological defects in space-time. According to Eq. (14), the topological charge of defects in two-dimensional crystal are conserved,

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot \vec{j} = 0. \]  

(24)

In addition, there is a constraint of ”charge neutrality”,

\[ \int \rho d^2x = \frac{1}{2\pi} \sum_{l=1}^{N} \beta_l \eta_l = 0. \]  

(25)

It indicate that the defect in two-dimensional crystal appear in pair.

Analogy to vortices in superfluid films, the zero point of the order parameter field play an important role in describing the topological defects in two-dimensional crystal. Now we study the properties of these zero points. If the Jacobian determinant $J^0(\phi_6/x) \neq 0$, we will have the isolated solution of the zeros of the order parameter field. But when $J^0(\phi_6/x) = 0$, the above results will change in some way, and will lead to the branch process of defects. We denote one of the vectors Jacobian at zero points as $(t^*, \vec{z}_l)$. According to the values of the vector Jacobian at zero points of the order parameter, there are limit points and bifurcation points. Each kind corresponds to different cases of branch processes.
FIG. 4: Two disclinations collide with different directions of motion at the bifurcation point in (2+1)-dimensional spacetime.

Let us explore what will happen to the disclination at the limit point \((t^*, \vec{z}_i^*)\). The limit points are determined by

\[
J^0 \left( \frac{\phi_6}{x} \right)_{t^*, \vec{z}_i^*} = 0, \quad J^1 \left( \frac{\phi_6}{x} \right)_{t^*, \vec{z}_i^*} \neq 0
\]  

(26)

\[
J^0 \left( \frac{\phi_6}{x} \right)_{t^*, \vec{z}_i^*} = 0, \quad J^2 \left( \frac{\phi_6}{x} \right)_{t^*, \vec{z}_i^*} \neq 0
\]  

(27)

Considering the condition (26) and making use of the implicit function theorem, the solution of Eq. (11) in the neighborhood of the point \((t^*, \vec{z}_i^*)\),

\[
t = t(x), \quad y = y(x)
\]  

(28)

where \(t^* = t(z_i^*)\). In this case, one can see that

\[
\frac{dx}{dt} \bigg|_{(t^*, \vec{z}_i^*)} = J^1 \left( \frac{\phi_6}{x} \right)_{J(\phi_6/x)} \bigg|_{(t^*, \vec{z}_i^*)} = \infty,
\]  

(29)

or

\[
\frac{dt}{dx} \bigg|_{(t^*, \vec{z}_i^*)} = 0.
\]  

(30)

The Taylor expansion of \(t = t(x)\) at the limit points \((t^*, \vec{z}_i^*)\) is

\[
t - t^* = \frac{1}{2} \frac{d^2 t}{dx^2} \bigg|_{t^*, \vec{z}_i^*} (x - z_i^*)^2,
\]  

(31)

which is a parabola in the x-t plane. From this equation, we can obtain two solutions \(x_1(t)\) and \(x_2(t)\), which give two branch solutions (World lines of disclinations). If

\[
\frac{d^2 t}{dx^2} \bigg|_{(t^*, \vec{z}_i^*)} > 0,
\]  

we have the branch solutions for \(t > t^*\). It is related to the origin of a disclination pair. Otherwise, we have the branch solutions for \(t < t^*\), which related to the annihilation of a disclination pair.

Since the topological current is identically conserved, the topological charges of these two generated or annihilated disclinations must be opposite at the limit points, say

\[
\beta_1 \eta_1 + \beta_2 \eta_2 = 0.
\]  

(32)

For a limit point it is required that \(J^1(\phi/x)_{t^*, \vec{z}_i^*} \neq 0\). As to bifurcation point, it must satisfy a more complex condition. This case will be discussed in the following.

Now, let us turn to consider in which the restrictions on zero point \((t^*, \vec{z}_i^*)\) are

\[
J^k \left( \frac{\phi_6}{x} \right)_{(t^*, \vec{z}_i^*)} = 0, \quad k = 0, 1, 2,
\]  

(33)

which imply an important fact that the function relationship between \(t\) and \(x\) or \(y\) is not unique in the neighborhood of the bifurcation point \((t^*, \vec{z}_i^*)\). This fact is easily seen from

\[
\frac{dx}{dt} = J^1 \left( \frac{\phi_6}{x} \right)_{J(\phi_6/x)} \bigg|_{t^*, \vec{z}_i^*}, \quad \frac{dy}{dt} = J^2 \left( \frac{\phi_6}{x} \right)_{J(\phi_6/x)} \bigg|_{t^*, \vec{z}_i^*},
\]  

(34)

which under Eq. (33) directly shows the indefiniteness of the direction of integral curve of Eq. (11) at \((t^*, \vec{z}_i^*)\). This is why the very point \((t^*, \vec{z}_i^*)\) is called a bifurcation point of the orientation order parameter.

With the aim of finding the different directions of all branch curves at the bifurcation point, we suppose

\[
\frac{\partial \phi_6}{\partial y} \bigg|_{t^*, \vec{z}_i^*} \neq 0.
\]  

(35)

According to the \(\phi\)-mapping theory, the Taylor expansion of the solution of the zeros of the order parameter field in the neighborhood of \((t^*, \vec{z}_i^*)\) can be expressed as

\[
A(x - z_i^*)^2 + 2B(x - z_i^*)(t - t^*) + C(t - t^*)^2 + ... = 0,
\]  

(36)
which leads to

\[ A \left( \frac{dt}{dx} \right)^2 + 2B \frac{dx}{dt} + C = 0, \]  

(37)

and

\[ C \left( \frac{dx}{dt} \right)^2 + 2B \frac{dt}{dx} + A = 0, \]  

(38)

where A, B, and C are constants determined by the order parameter. The solutions of Eq. (37) or Eq. (38) give different directions of the branch curves (world line of vortices) at the bifurcation point. There are four possible cases, which will show the physical meanings of the bifurcation points.

Case 1 \((A \neq 0)\). For \(\Delta = 4(B^2 - AC) > 0\), from Eq. (37) we get two different motion directions of the core of disclination

\[ \frac{dx}{dt} \bigg|_{1,2} = \frac{-B \pm \sqrt{B^2 - AC}}{A}, \]  

(39)

where two world lines of two disclination intersect which different directions at the bifurcation point. This shows that two disclinations encounter and the depart at the bifurcation point.

Case 2 \((A \neq 0)\). For \(\Delta = 4(B^2 - AC) > 0\), form Eq. (37), we obtain only one motion direction of the core of disclination

\[ \frac{dx}{dt} \bigg|_{1,2} = \frac{-B}{A}, \]  

(40)

which includes three important cases. (i) Two world lines tangentially contact, i.e., two disclinations tangentially encounter at the bifurcation point. (ii) Two world lines merge into one world line, i.e., two disclinations merge into one disclination at the bifurcation point. (iii) One world line resolves into two world lines, i.e., one disclination splits into two disclinations at the bifurcation point.

Case 3 \((A = 0, C \neq 0)\). For \(\Delta = 4(B^2 - AC) = 0\) from Eq. (37) we have

\[ \frac{dt}{dx} \bigg|_{1,2} = \frac{-B \pm \sqrt{B^2 - AC}}{C} = 0, \quad -\frac{2B}{C}. \]  

(41)

There are two important cases: (i) One world line resolves into three world lines, i.e., one disclination split into three disclinations at the bifurcation point. (ii) Three world line merge into one world line, i.e., three disclinations merge into one disclination at the bifurcation point.

Case 4 \((A=C=0)\). Equations (37) and (38) give respectively

\[ \frac{dx}{dt} = 0, \quad \frac{dt}{dx} = 0. \]  

(42)

This case shows that two worldlines intersect normally at the bifurcation point, which is similar to case 3. It is no surprise that both parts of Eq. (42) are correct because they give the slope coefficients of two different curves at the same point \((t^*, \vec{z})\).

In conclusion, we study the inner topological structure of disclinations in two-dimensional colloidal systems. We have obtained a more essential topological formulay of charge density of disclinations in two-dimensional crystals, and revealed the inner topological relationship of the charge of disclinations is characterized by the Hopf index and the Brouwer degree. We have studied the evolution of disclinations by making use of Duan’s topological current theory. We concluded that there exist crucial cases of branch processes in the evolution of disclinations when \(J(\phi/x) = 0\), i.e., \(\eta_l\) is indefinite. It means that disclinations are generated or annihilated at the limit points and are encountered, split, or merge at the bifurcation points, which shows that the disclination is unstable at these branch points. We would like to pointed that all the results in this paper obtains from the viewpoint of topology without any hypothesis, and they are not depended on the property of systems, such as interaction between particles.

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