The Topological Origin of the Peierls-Nabarro Barrier

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Crystals and other condensed matter systems described by density waves often exhibit dislocations. Here we show, by considering the topology of the ground state manifolds (GSMs) of such systems, that dislocations in the density phase field always split into disclinations, and that the disclinations themselves are constrained to sit at particular points in the GSM. Consequently, the topology of the GSM forbids zero-energy dislocation glide, giving rise to a Peierls-Nabarro barrier.

The symmetries of crystals are encoded by groups: the space group of each possible crystalline arrangement is composed of discrete translations, rotations, glides, mirrors, and screws that form finite subgroups of the Euclidean group in the dimension of interest. As a result, and as strikingly measured in X-ray diffraction, physical crystals provide a near Platonic manifestation of rigid geometry via their periodicities. These symmetries are encoded in the ground state manifold (GSM) that parameterizes degenerate ground states. The coordinates of the GSM are the Nambu-Goldstone modes of the system – the zero-energy deformations. When the GSM is spanned by these modes (moduli), homotopy theory allows for the classification of topological defects. For instance, the discrete translational symmetry of the crystal leads to dislocations with “charges” that are integer combinations of the lattice basis vectors – the Burgers vector. In the classic discussion by Peierls, the dislocations move in the background of the lattice and it follows that an energy cost associated with Peierls, the dislocations move in the background of the lattice and it follows that an energy cost associated with the motion of particles is incurred: the Peierls-Nabarro barrier.

What happens, however, when the crystal is very soft? As a concrete example, recall the Tonks-Girardeau cation motion is based. The “Nabarro-Peierls” barrier is the keystone upon which dislocation glide inherits the crystal periodicity. The “Nabarro-Peierls” barrier is the keystone upon which dislocation glide inherits the crystal periodicity. The “Nabarro-Peierls” barrier is the keystone upon which dislocation glide inherits the crystal periodicity. The “Nabarro-Peierls” barrier is the keystone upon which dislocation glide inherits the crystal periodicity.

Figure 1. Left: The two-dimensional smectic GSM (Klein bottle) featuring a path corresponding to a dislocation (red) winding in φ. The dashed blue line is at φ = π and along with the vertical at φ = 0 comprise the allowed disclination locations. Right: Decomposition of dislocations into disclinations in the GSM. The red path is deformed, employing the equivalence relations for the Klein bottle the segments γ2 and γ4 are now identical but with opposite orientation. The remaining segments γ1 and γ3 correspond to disclinations at a density maximum (∠φ = 0) and minimum (∠φ = π) respectively – the dislocation has been decomposed into a pair of disclinations as shown in the upper left of Fig. 2. This defect complex does not require δρ to vanish anywhere.

The symmetries of crystal in order to introduce disclinations along with the dislocations. As noted in, homotopy theory fails to characterize these defects because the Nambu-Goldstone moduli do not span the GSM. As discussed in, this can be resolved via the use of Morse-theoretic tools. Specifically, between two maxima in the density wave, reflected in X-ray diffraction, there must be saddles and minima. These critical points, on the same lengthscale as the Peierls potential, are the essence of the topological barrier.

We first consider the two-dimensional smectic which captures the essence of this work. The layer structure of the smectic ground state can be described by the phase field Φ = k ⋅ x + φ. The density is reconstructed via ρ = ρ0 + δρ cos Φ, the layers sit on density maxima (cos Φ = 1).
to a point, if we were to contract the measuring path in the sample, $\phi$ must approach a constant limiting value in the GSM. But the condition on the GSM $(0, \phi) \cong (\pi, -\phi)$ implies that this constant value of $\phi$ must satisfy $\phi \cong -\phi$, so $\phi = 0$ or $\pi$. Hence $\pm \pi$ disclinations in smectics must sit on density minima/maxima [10] [11]. We can also see that only these values of $\phi$ allow a pure disclination – other values of $\phi$ would prevent the loop from closing in the GSM. Recall that the smectic groundstate has a single Goldstone mode, arising from the zero-energy deformation $\phi \mapsto \phi + \epsilon$, indeed this deformation is a zero energy translation for any defect-free smectic configuration and amounts to shifting the origin. However, in the presence of disclinations it is no longer possible to make the transformation $\phi \mapsto \phi + \epsilon$, since the value of $\phi$ on disclinations is topologically fixed. In other words, the presence of disclinations implies the smectic energy no longer has a $U(1)$ symmetry. In particular, de Gennes’ model of the smectic [16] cannot accurately describe disclinations [12] [13].

How does this affect dislocations? Dislocations are necessarily made of a topologically protected arrangement of disclinations with zero net charge. This follows because lines of phase maxima must be separated by lines of phase minima [11]. In the GSM a charge one dislocation is represented by a path winding $2\pi$ in $\phi$ (Fig. 1 left), by manipulating the path, using the topology of the Klein bottle, it is converted in to two disclinations, one on a density maximum and one on a density minimum (Fig. 1 right); the real-space realisation is shown in Fig. 2 (top left). By including more maxima/minima lines, we can increase the charge by changing the “length” of the disclination dipole. Alternatively, one could, for instance, attempt to construct a charge two dislocation out of a $\pm 2\pi$ disclination pair. However, because $+2\pi$ disclinations cannot connect to distant layers, it is necessary to balance the $-2\pi$ disclination with two $\pi$ disclinations. As there are no disclinations with charge higher than $2\pi$ [5] it follows that all dislocations must contain $\pi$ disclinations on either a phase maximum or minimum. Thus, purely on symmetry grounds, a dislocation glide is forbidden by the topology of the GSM: the Peierls-Nabarro barrier. Indeed, in order for a dislocation to glide, the smectic order itself must melt, allowing the disclinations to hop from one layer to another, moving from one topological sector to another.

We now extend this discussion to the five Bravais latices describing two-dimensional crystals, beginning with a description of the GSM. A two-dimensional lattice is determined by two basis vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ with reciprocal lattice vectors $\mathbf{k}_1$ and $\mathbf{k}_2$, $\mathbf{k}_i \cdot \mathbf{e}_j = \delta_{ij}$. In a two-dimensional lattice, the vertices can be specified by maxima of $\cos \Phi_1 + \cos \Phi_2$ where the two phase fields are $\Phi_i = \mathbf{k}_i \cdot \mathbf{x} + \phi_i (i = 1, 2)$. Reusing $\theta$ to specify the orientation of the lattice with respect to a fixed-axis, the GSM
Since we know a translation of which is equivalent to a rotation about the origin by symmetry of the lattice. Applying the rotation gives suppose that a rotation by This symmetry allows us to choose vector is a symmetry of the lattice, so corresponding to $x_0$ is (minus) the position vector of the lattice point. This symmetry allows us to choose $x_0$ in the unit cell. Now, suppose that a rotation by $\theta_0$, denoted $R$, about $-x_0$ is a symmetry of the lattice. Applying the rotation gives which is equivalent to a rotation about the origin by $R$ and a translation of $\phi_i$ by $[(1 - R)k_i] \cdot x_0$.

Since we know $\Phi_i \cong \Phi'_i$, we find the equivalence relation

$$ (\theta, \phi_1, \phi_2) \cong \left( \theta + \theta_0, (Rk_1) \cdot x_0, (Rk_2) \cdot x_0 \right), $$

with $\phi_i = k_i \cdot x_0$. Along with the translational symmetry, this specifies the GSM for the two-dimensional Bravais lattices. The basic rotational symmetries of the five Bravais lattices are $\theta_0 = \pi$ for the oblique (O), rectangular (R) and centered rectangular (CR), $\pi/2$ for the square (S), and $\pi/3$ for the triangular (T), in each case we obtain a topologically distinct GSM, as shown in Fig. and listed in Tab. I. These can be described topologically as the product of a unit cell (a torus) with the interval $[0, \theta_0]$, such that the 0 and $\theta_0$ unit cells are glued together with a $\theta_0$ twist. Formally, this defines an element of $SL(2, \mathbb{Z})$, a new choice of basis vectors, for the closed path from 0 to $\theta_0$. The matrices for $\theta_0 = \pi, \pi/2, \pi/3$ are of finite orders 2, 4, and 6, corresponding to the allowed point groups of a lattice without basis. Finally, It should be noted that although the function $\cos \Phi_1 + \cos \Phi_2$ is sufficient to describe the symmetries of the lattice via maxima points, it is not guaranteed that the density field has the same symmetry. This is only an issue in the triangular lattice. In order to have the density enjoy the full, six-fold symmetry around each lattice point we must assign a third phase field $\Phi_3 \cong -\Phi_1 - \Phi_2$ (for the convention of $k_1, k_2$ differing by angle $2\pi/3$), and promote

| Lattices | $\theta_0$ | GSM $(\theta, \phi_1, \phi_2) \cong$ | Disclination Angles | GSM Locations |
|----------|------------|----------------------------------|---------------------|---------------|
| O, R, CR | $\pi$      | $(\theta + \pi, -\phi_1, -\phi_2)$ | $\pm \pi$           | $(0, 0) (0, \pi) (0, \pi)$ |
| S        | $\pi/2$    | $(\theta + \pi/2, \phi_2, -\phi_1)$ | $\pm \pi/2$         | $(0, 0) (0, \pi)$          |
| T        | $\pi/3$    | $(\theta + \pi/3, \phi_1 + \phi_2, -\phi_1)$ | $\pm 2\pi/3$        | $(0, 0) (2\pi/3, 2\pi/3) (4\pi/3, 4\pi/3)$ |

Table I. Groundstate manifolds (GSMs), disclinations and their GSM locations for the oblique (O), rectangular (R), centered rectangular (CR), square (S), triangular (T).
the vicinity of a defect there can be no consistent labelling of $\Phi_1$ and $\Phi_2$. Despite this, dislocations still split into phase disclinations as before, as shown in Fig. 4. Despite the seemingly ambiguous nature of the phases around a disclination, when a measuring path is mapped to the GSM no such discontinuity is seen, since the GSM is the space of states modulo equivalent states; disclinations $\{d_i\}$ in a lattice $\Omega$ correspond to a smooth map $f: \Omega/\{d_i\} \to GSM$. In a manner directly analogous to the smectic, the topology of the GSM dictates the locations of phase disclinations. Consider shrinking the radius of a measuring loop around a disclination, such that $\phi_1$ and $\phi_2$ approach constant values, but $\theta \to \theta + n\theta_0$. This can then only occur at locations in the GSM where $(\phi_1, \phi_2)$ is invariant under $\theta \to \theta + n\theta_0$, so that $\exists a, b \in \mathbb{Z}$ such that

$$R_{\pm \theta_0} \left( \begin{array}{c} \phi_1 \\ \phi_2 \end{array} \right) = \left( \begin{array}{c} \phi_1 \\ \phi_2 \end{array} \right) + \frac{2\pi a}{2\pi b} \left( \begin{array}{c} \pi \theta \\ \pi \phi \end{array} \right)$$

(5)

Consider the square lattice as an example, we have seen the twisting of the GSM is described by $(\theta, \phi_1, \phi_2) \cong (\theta + \pi/2, \phi_2, -\phi_1)$. This has solutions when $\phi_1$ and $\phi_2$ are both minima or both maxima: the disclinations are confined to one of two positions within the unit cell, here corresponding to crystal disclinations lying on vertices of the lattice or dual lattice. The full list of allowed phase disclination densities is given in Tab. 1. There we see that the standard “5” and “7” disclinations of the triangular lattice always lie on double maxima – in agreement with the classic theory of crystal disclinations employed in two-dimensional melting [17–19]. We note that in the square and triangular lattices, disclinations of higher winding than the elementary $\pi/2$ or $\pi/3$ may exist – the lower symmetry gives such disclinations greater freedom of location.

Since phase disclinations must lie on a restricted set of points in the unit cell in order for the phase field to be continuous, it follows that there is a Peierls-Nabarro barrier for dislocations that must contain disclinations; the ground state symmetry immobilises the underlying disclination structure of a lattice dislocation. A dislocation cannot glide without first melting the density wave order. This is akin to closing the mass gap in topological insulators: in order to transition from one topological sector to the other the density wave must vanish, destroying the ability to define the phase fields $\Phi_i$ and allowing topological invariants to “tunnel” from one value to another [20].

We have shown that in two-dimensions the Peierls-Nabarro barrier follows from topological considerations. What happens in three-dimensions? In this case disclinations and dislocations are described by lines or closed loops in the sample, not points. In cross section, perpendicular to the defect lines, our arguments continue to hold and there remains a topological Peierls-Nabarro barrier to glide. However, when the defect lines bend, there are likely to be further, global, topological constraints as there are...
in, for instance, biaxial nematics [1], cholesterics [21, 22], and smectics [11, 23]. Whether these additional constraints can be resolved or lead to additional topological invariants remains an open question.

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