Disclination Loop Critical Behavior in Nematic Liquid Crystals

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- Defect-mediated transitions in ferromagnets
- Defects in nematics
- Simulations: Lebwohl-Lasher type models
- Conclusions
Two-dimensional XY model

- Order parameter: two-dimensional vector
- Topological defects: points (vortices) indexed by positive and negative integers
- Kosterlitz-Thouless theory:
  
  - Below $T_{KT}$ vortices are bound in pairs of zero net charge
  - Above $T_{KT}$ vortex pairs begin to unbind; unbound vortices lead to disorder
Three-dimensional XY model

- Defects: *lines* which form closed loops or terminate on system boundaries
- Loops are "directed" like $\vec{J}$ in current carrying loops: the local tangent describes the sense of the circulation of the spins
- Loops have no net "monopole" charge
Can defect loops mediate the 3d XY transition?

- On general theoretical grounds, yes!
- But, there's no theory comparable to KT.
- Numerical evidence (Nguyen and Sudbo):
  - Loop distribution function: average number of loops with perimeter $p$
    \[ D(p) = p^{-\alpha} \exp(-\varepsilon(T)p / k_B T) \]
    \[ \varepsilon(T) = \text{defect line tension } \neq 0, T < T_c \]
  - Probability $O_L$ of defect line crossing the sample,
    \[ O_L = 0, T < T_c \]
Nguyen and Sudbo: 3d XY Model

\[ D(p) = p^{-\alpha} \exp\left(-\varepsilon(T)p / k_B T\right) \]
What about the 3d Heisenberg model?

- Order parameter: three-dimensional vector
- Topological defects: points ("monopoles", "hedgehogs") of integral charge
- Simulations by Lau and Dasgupta suggest that monopoles mediate the transition
- Suppressing the monopoles eliminates the transition, leaving the system ordered.
Defects in Nematic Liquid Crystals

Nematics can have:

- disclination lines of half integer charge

forming loops or terminating on boundaries

- monopoles like the Heisenberg model, though positive and negative charges are equivalent
Some loops can carry monopole charge

Twist loop (no monopole charge): rotation vector $\Omega$ is perpendicular to the loop plane

$$\Omega \perp \overline{\Omega} \left( \ell \right) dl = \pi \hat{z}$$

Wedge loop (unit monopole charge): rotation vector $\Omega$ is locally parallel to the disclination line:

$$\Omega \parallel \overline{\Omega} \left( \ell \right) dl = 0$$

- Wedge loops look like monopoles at large distances
- Twist loops yield a uniform director structure; they have no net topological charge (just like the loops in the 3d XY model)
Monopole charge of loops: more generally

\[ \frac{1}{p} \int \mathbf{\Omega}(\ell) d\ell = 0 \quad \text{the loop carries a monopole charge} \]
Questions:

• Which of the topologically permissible defects do in fact appear?

• What are the relative populations of these defects?

• What role do the defects play at the phase transition?

• How do the defects influence the order of the transition?
Lammert, Rokhsar and Toner

\[ H = -J \sum_{ij} U_{ij} \sigma_i \bar{\sigma}_j - K \sum U_{ij} U_{jk} U_{kl} U_{li} \]

\[ \sigma_i \]

\[ \begin{array}{ll}
\text{K} = 0:\text{ trace over } U \Rightarrow \text{ Lebwohl-Lasher for small } J \\
\text{K} \to \infty: \text{ disclination lines are suppressed, but not the monopoles } \Rightarrow \text{ Heisenberg model}
\end{array} \]
Lammert, Rokhsar and Toner

- Generalized Lebwohl-Lasher (lattice) model of nematics
- If disclination lines are suppressed (but not monopoles), the NI transition becomes more continuous
- Suppress disclination lines completely: Heisenberg model
Our work: simulations of the Lebwohl-Lasher and related models

\[ H = -J \sum_{<ij>} \left\{ \frac{3}{2} (\vec{\sigma}_i \cdot \vec{\sigma}_j)^2 - \frac{1}{2} \right\} \]

We used a “cluster” MC algorithm which is much more efficient than the ordinary single “spin flip” algorithm in the critical region.

System sizes up to \( 70^3 \) were simulated.
Modified Lebwohl-Lasher

\[ H = -J \sum_{\langle ij \rangle} P_2(\vec{\sigma}_i \cdot \vec{\sigma}_j) - J' \sum_{\langle ij \rangle} P_4(\vec{\sigma}_i \cdot \vec{\sigma}_j) \]

As shown by Zannoni et al. (using mean-field theory and Monte Carlo), this model has a first order transition whose strength increases with increasing \( J' \).
Comparing potentials: $P_2(x)$ and $P_2(x)+0.3P_4(x)$, $x = \bar{\sigma}_i \bar{\sigma}_j$
Defect-finding Algorithms

Disclinations (Zapotocky, Goldbart & Goldenfeld)

\[ \sigma_A \]

Mapping \[ A \rightarrow B \rightarrow C \rightarrow D \]

Order parameter sphere

Track the director on the order parameter (OP) sphere while moving around a lattice square (\( A \rightarrow B \rightarrow C \rightarrow D \)). Choose \( \sigma \) or \(-\sigma\) so that the shortest arc length is obtained. Compare \( \sigma_D \) with \( \sigma_A \). If these two are closer to each other than \(-\sigma_D\) and \(\sigma_A\), there is no defect; otherwise there’s a half-integer disclination line passing through the plaquettes.
Heisenberg Monopoles (Berg-Luscher)

Divide each of the lattice cube faces into 2 triangles. Map the directors at the corners of each of the 12 triangles to the OP sphere (using shortest "distance").

Sum the signed $\text{sgn}(\vec{\sigma}_A \cdot (\vec{\sigma}_B \times \vec{\sigma}_C))$ areas of the 12 surfaces formed on the OP and divide by $4\pi$; this yields the integer-valued topological charge.

Eight directors is not sufficient for nematic monopoles (Hindmarsh)
Monopole Charge of Loops

- Direct measurement: apply Berg-Luscher method to the surface of a set of lattice cubes surrounding the loop.
- Alternatively: Compute the rotation vector $\Omega$ of the director around the plaquette by summing the cross products of each neighboring pair of directors:

$$\tilde{\Omega} = (\vec{\sigma}_i \times \vec{\sigma}_j) + (\vec{\sigma}_j \times \vec{\sigma}_k) + (\vec{\sigma}_k \times \vec{\sigma}_l) + (\vec{\sigma}_l \times (-\vec{\sigma}_i))$$

- Recall: If $\frac{1}{p} \int \tilde{\Omega}(l) dl = 0$ then the loop has monopole charge
Free energy

\[ F = - \ln P(E) \]

\[ L = 70, \ T_{NI} = 1.1226 \]

Smaller system size L
"Free energy" as a function of disclination line segments

-\ln P(\rho)

\[ L = 70, \ T_{\text{NI}} = 1.1226 \]
Loop distribution: Lebwohl-Lasher

- System size: $70^3$
- $T_{NI}$ coincides with equal well depths in the free energy
- $\varepsilon(T_{NI}) \approx 0$, $\varepsilon(T<T_{NI}) = 0.01$

\[ D(p) = p^{-\alpha} \exp(-\varepsilon(T)p / k_B T) \]

$\alpha \approx 2.5 \pm 0.1$
Loop distribution: $P_4$ model
$J^\prime/J = 0.3$, $T = T_{NI} = 1.2475$

$$D(p) = p^{-\alpha} \exp(-\varepsilon(T) p / k_B T)$$
$$\alpha \approx 2.5, \varepsilon(T_{NI}) \approx 0.002$$

System size $50^3$

Isotropic phase
Nematic phase
Monopoles

We found *no* point monopoles in either model (there are topological arguments due to Hindmarsh suggesting that monopoles are rare).
Monopole loop charge: $\frac{1}{p} \int \vec{\Omega}(\ell) d\ell$
Conclusions

- Disclination loops “blow out” at the NI transition in a discontinuous way if the transition is strongly first order
- No point monopoles are observed
- Loops can carry monopole charge, and there are large loops with charge
- The order of the transition does not appear to correlate with the nature of the defects

Order parameter sphere

Mapping of directors around an infinitesimal loop segment

Planar loop

\[ \Theta = \pi/2, \text{ wedge loop}; \quad \Theta = 0, \text{ twist loop} \]