Disclination Loop Critical Behavior in Nematic Liquid Crystals

N.V. Priezjev
R. A. Pelcovits

Phys. Rev. E **64,** 031710 (2001)

- **Defect-mediated transitions in ferromagnets**
- **Defects in nematics**
- **Simulations: Lebwohl-Lasher type models**
- **Conclusions**

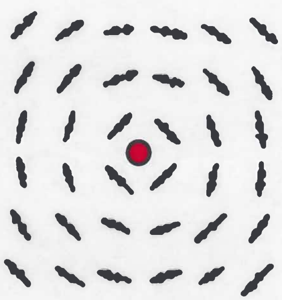
Brown Physics

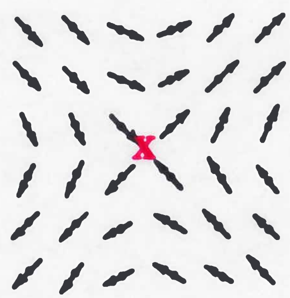
Two-dimensional XY model

- 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





Brown Physics

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

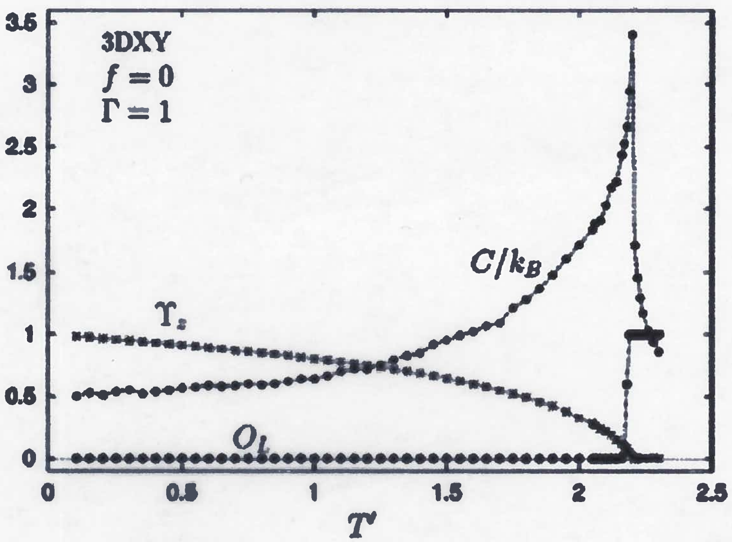
$$D(p) = p^{-\alpha} \exp(-\varepsilon(T)\, p / k_B T)$$

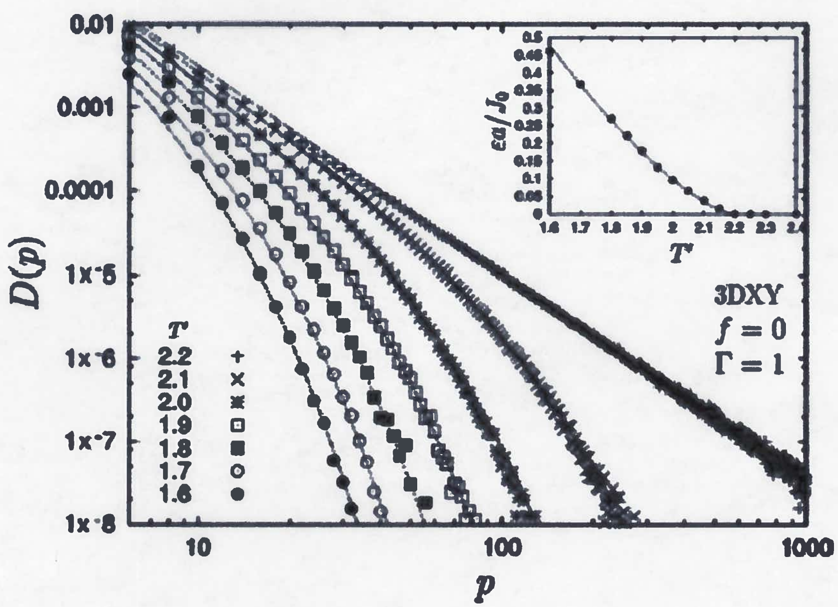
$$\varepsilon(T) = \text{defect line tension} \neq 0, \mathrm{T} < \mathrm{T_c}$$

  - Probability O_L of defect line crossing the sample, $O_L = 0$, $\mathrm{T} < \mathrm{T_c}$

Brown Physics

Nguyen and Sudbo: 3d XY Model





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

Brown Physics

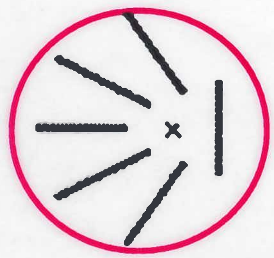
What about the 3d Heisenberg model?

- 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

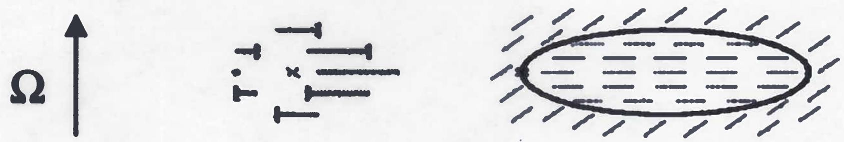


  forming loops or terminating on boundaries

- 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 Ω is perpendicular to the loop plane



$$\frac{1}{p}\int \vec{\Omega}(\ell)\,d\ell = \pi\hat{z}$$

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

$$\frac{1}{p}\int \vec{\Omega}(\ell)\,d\ell = 0$$

- **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)**

Brown Physics

Monopole charge of loops: more generally

If $\frac{1}{p}\int \vec{\Omega}(\ell)d\ell = 0$ the loop carries a monopole charge

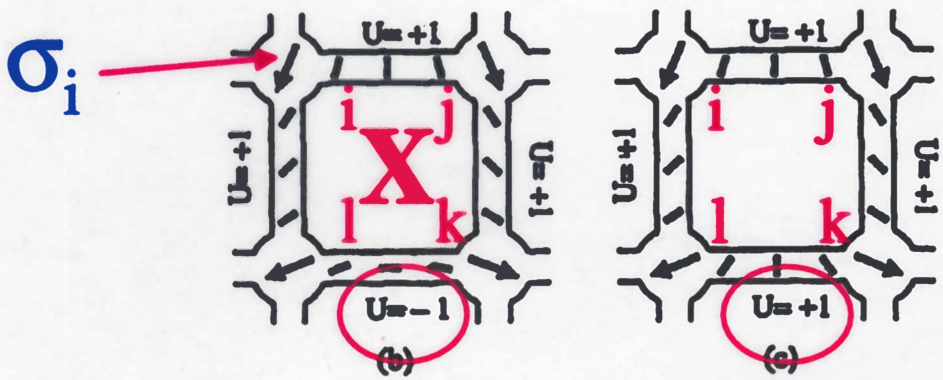
Brown Physics

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

$$H = -J \sum_{<ij>} U_{ij} \vec{\sigma}_i \cdot \vec{\sigma}_j - K \sum_{\square} U_{ij} U_{jk} U_{kl} U_{li}$$



K = 0: trace over U ⇒ Lebwohl-Lasher for small J

K → ∞: disclination lines are suppressed, but not the monopoles ⇒ Heisenberg model

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.

Brown Physics

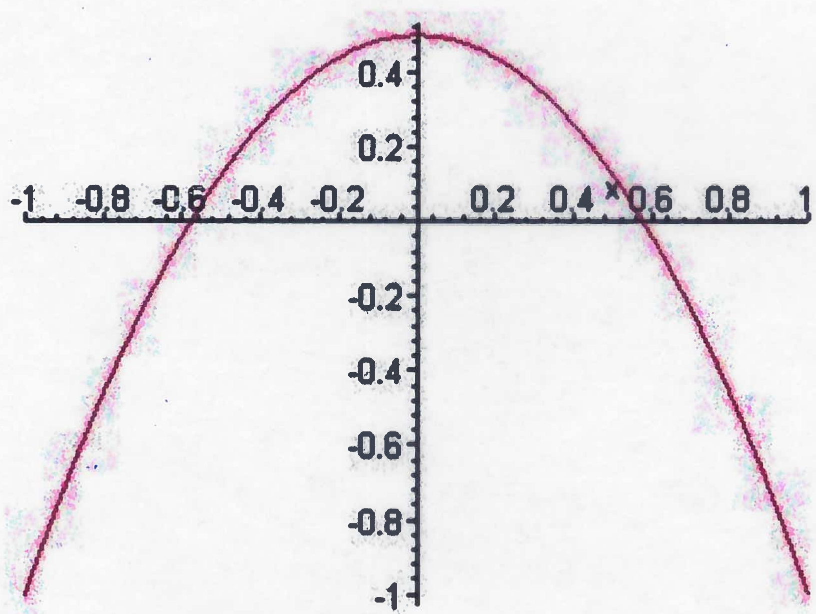
Modified Lebwohl-Lasher

$$H = -J\sum_{<ij>} P_2(\vec{\sigma}_i \cdot \vec{\sigma}_j) - J'\sum_{<ij>} P_4(\vec{\sigma}_i \cdot \vec{\sigma}_j)$$

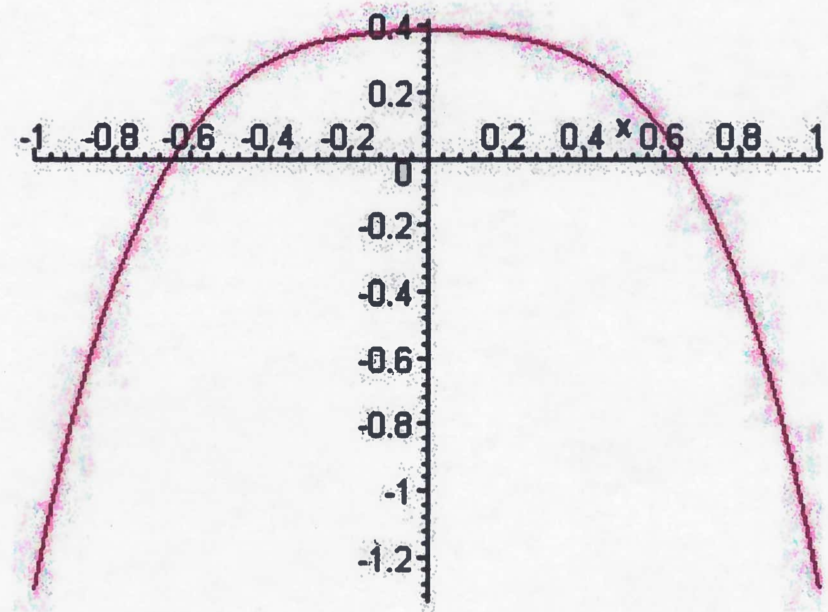
As shown by Zannoni et al. (using mean-field theory and Monte Carlo), this model has a first order transition whose strength increases with increasing J´

Brown Physics

Comparing potentials: $P_2(x)$ and $P_2(x)+0.3P_4(x)$, $x=\vec{\sigma}_i \cdot \vec{\sigma}_j$



P_2

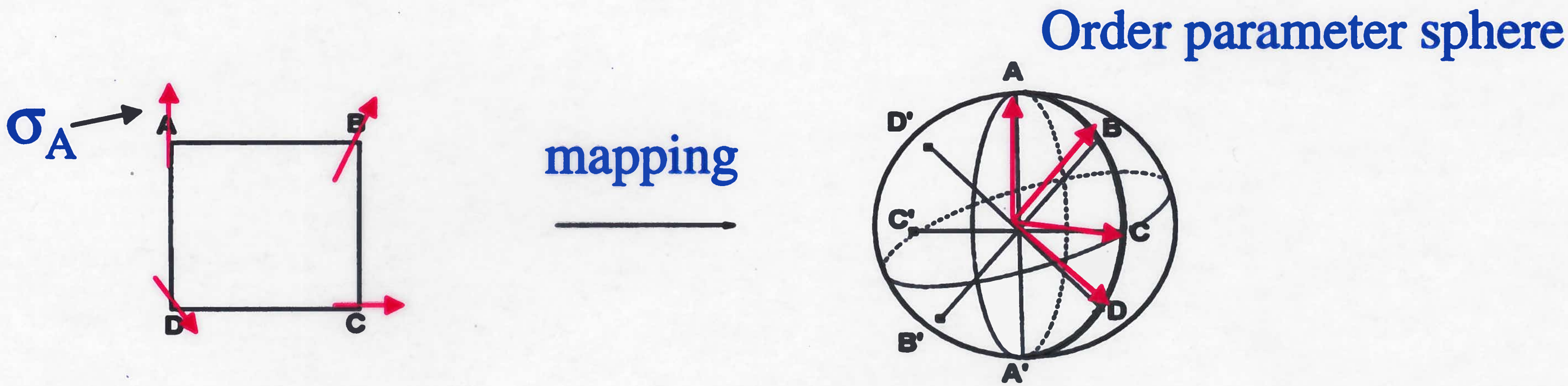


$P_2+0.3P_4$

Brown Physics

Defect-finding Algorithms

Disclinations (Zapotocky, Goldbart & Goldenfeld)

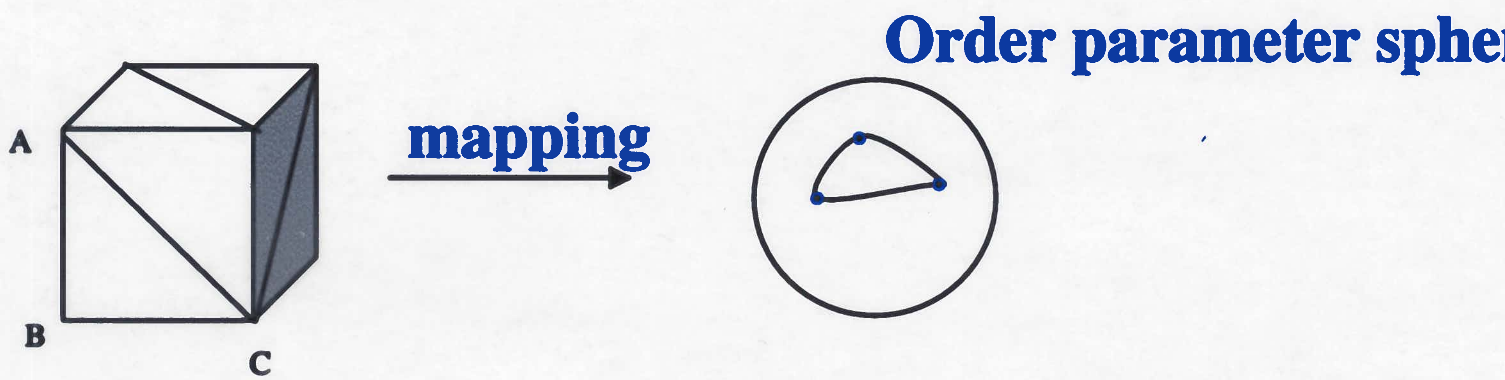


Track the director on the order parameter (OP) sphere while moving around a lattice square (A→B→C→D). Choose σ or $-\sigma$ so that the shortest arc length is obtained. Compare σ_D with σ_A. If these two are closer to each other than $-\sigma_D$ and σ_A, there is no defect; otherwise there's a half-integer disclination line passing through the plaquette.

Brown Physics

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



Eight directors is *not* sufficient for nematic monopoles (Hindmarsh)

Brown Physics

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 Ω of the director around the plaquette by summing the cross products of each neighboring pair of directors:**

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

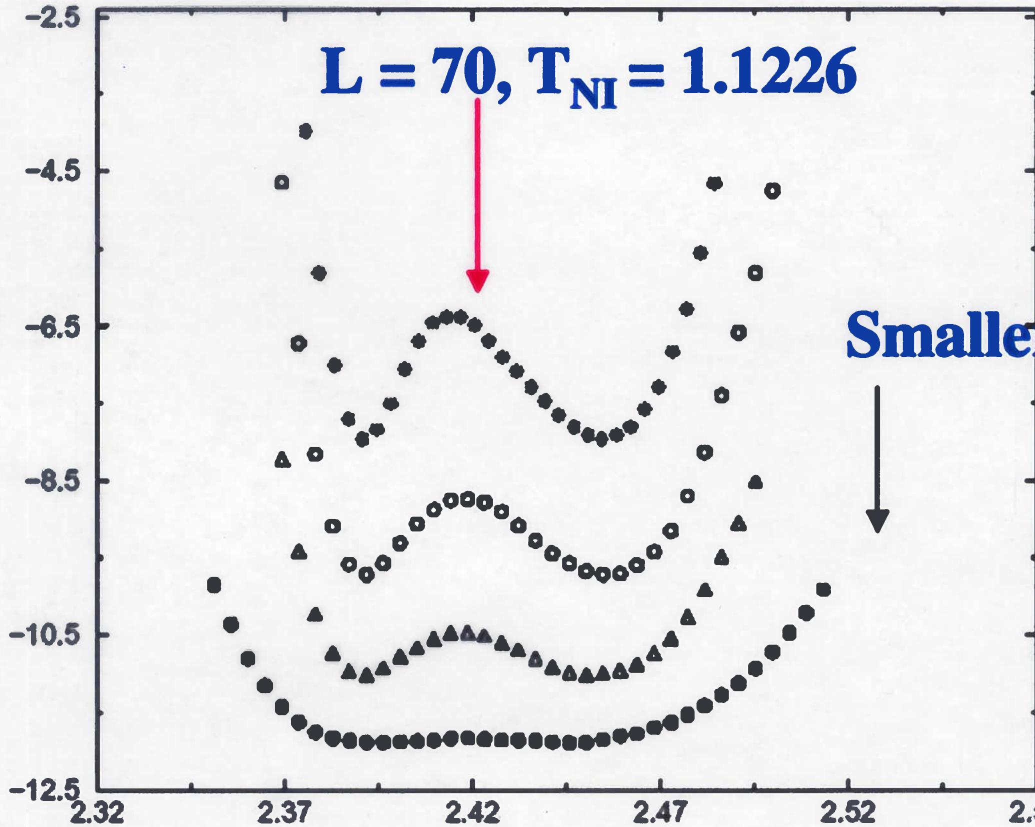
- **Recall: If** $\frac{1}{p}\int \vec{\Omega}(\ell)\, d\ell = 0$ **then the loop *has* monopole charge**

Brown Physics

Priezjev & Pelcovits, Phys. Rev. E **63,** 062702 (2001)

Free energy

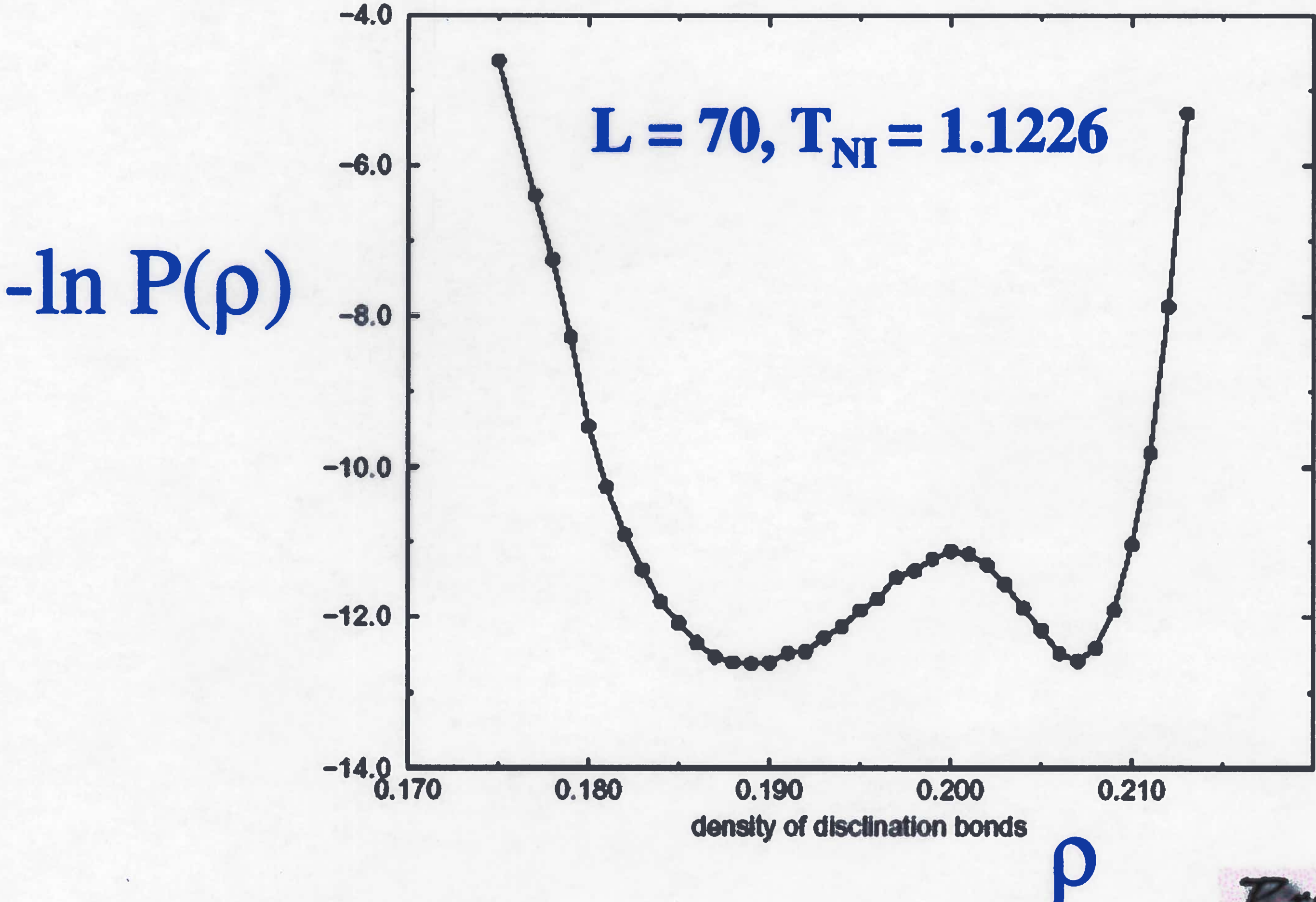
$F = -\ln P(E)$



Smaller system size L

-E

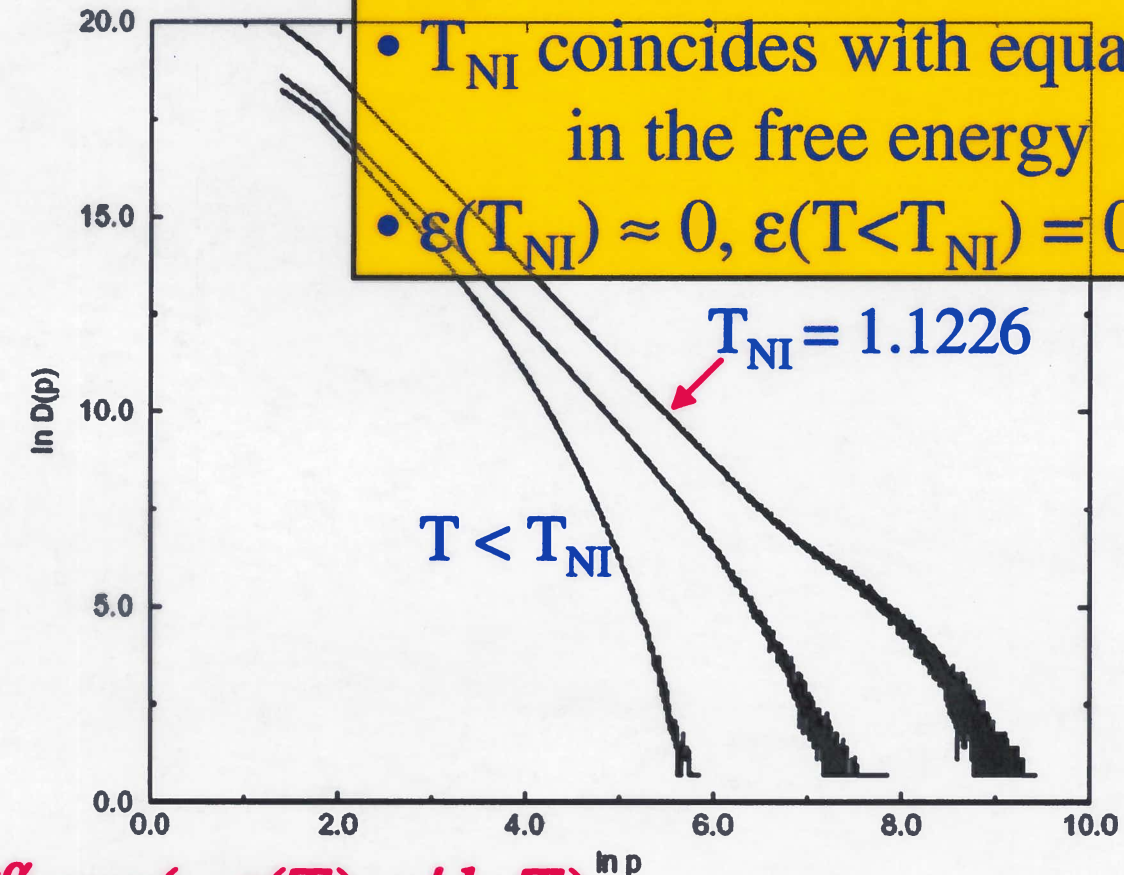
"Free energy" as a function of disclination line segments



Brown Physics

Loop distribution: Lebwohl-Lasher

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

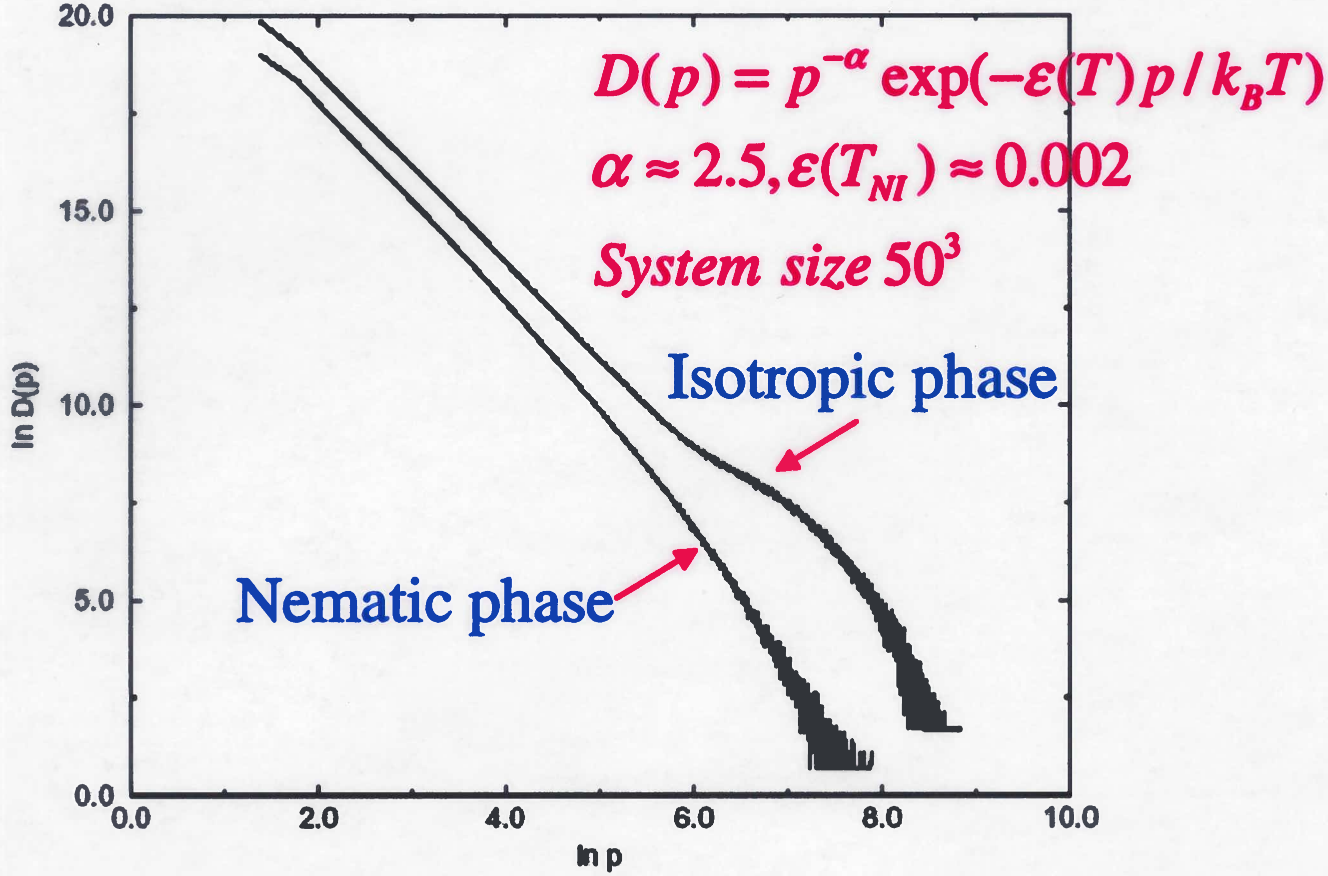


$$D(p) = p^{-\alpha}\exp(-\varepsilon(T)p/k_BT)$$

$$\alpha \approx 2.5 \pm 0.1$$

Brown Physics

Loop distribution: P_4 model
$J'/J = 0.3$, $T = T_{NI} = 1.2475$

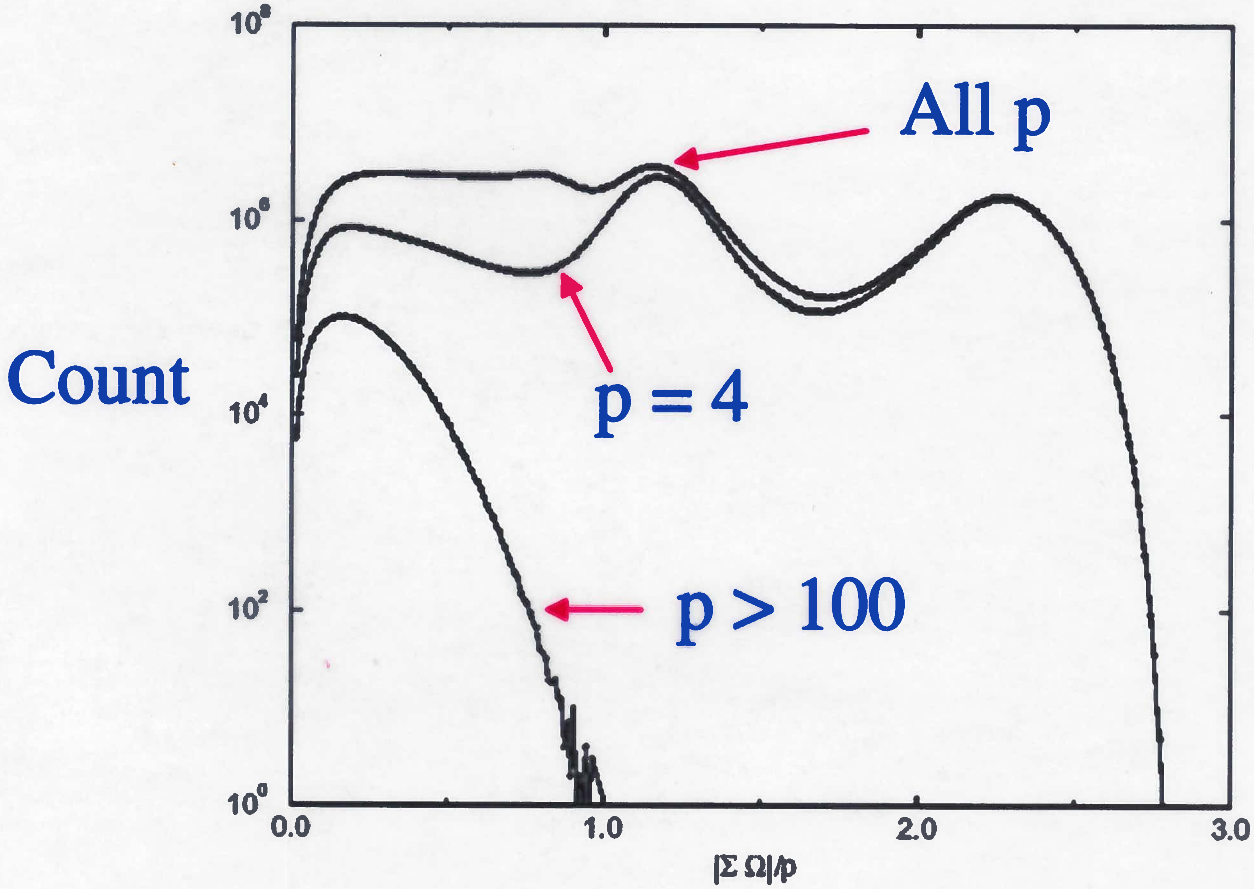


Brown Physics

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

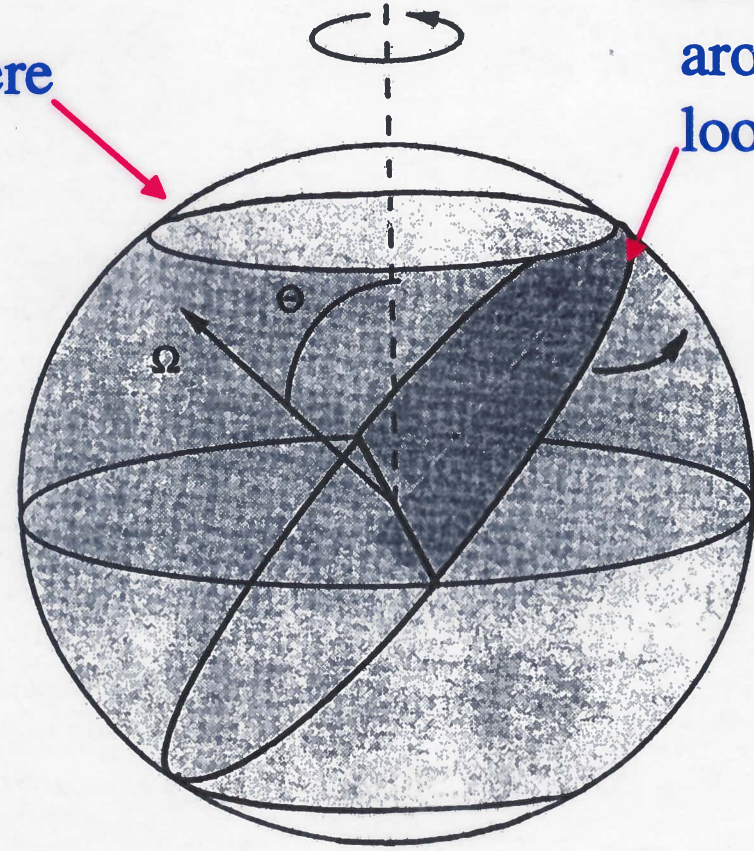
- Disclination loops "blow out" at the NI transition in a discontinuous way if the transition is strongly first order
- No point monopoles are observed
- Loops can carry monopole charge, and there are *large* loops with charge
- The order of the transition does *not* appear to correlate with the nature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

Terentjev, Phys. Rev. E 51, 1330 (1995)

Order parameter sphere

Mapping of directors around an infinitesimal loop segment

Planar loop



$\Theta = \pi/2$, wedge loop; $\Theta = 0$, twist loop

Brown Physics