Lebwohl-Lasher models of liquid crystals: from quadrupolar to spontaneously induced chiral order

Lech Longa (Kraków, Poland)
Karol Trojanowski
Grzegorz Pająk

Jagiellonian University
Marian Smoluchowski
Institute of Physics
The Lebwohl- Lasher model
(Lattice Liquid Crystals)

Single-site soft potentials:

\[ V = -\varepsilon \sum_{<ij>} \left( \frac{3}{2} \cos^2 \theta_{ij} - \frac{1}{2} \right) \equiv -\varepsilon \sum_{<ij>} P_2(\cos \theta_{ij}) \]

\[ V_{ij} = -\varepsilon \quad Q_{U,i} \cdot Q_{U,j} = -\varepsilon \]

1. **Mayer-Saupe** uniaxial quadrupoles are assumed to occupy the sites of a three dimensional cubic lattice.
2. **Model preserves nematic symmetry** \((D_{\infty h})\).
3. No dependence on the orientation of the radius vector connecting molecular centers.
4. **Orientational structures identified not only characterize nematic-like states but can also coexist with a long-range positional order, characteristic of smectic, columnar or crystalline phases.**
Lebwohl- Lasher model
(results, 3d cubic lattice)

\[ V = -\epsilon \sum_{<i,j>} \left( \frac{3}{2} \cos^2 \theta_{ij} - \frac{1}{2} \right) \equiv -\epsilon \sum_{<i,j>} P_2(\cos \theta_{ij}) = -\frac{3}{2} \epsilon \sum_{<i,j>} (i_3 \cdot j_3)^2 + \text{const} \]

\[
\begin{array}{cccc}
\text{Monte Carlo}^a & \text{Mean field (Maier-Saupe)} & \text{Two-cluster mean field}^b & \text{Four-cluster mean field}^c \\
T_{NI}/\epsilon_0 & 1.127 & 1.321 & 1.160 & 1.142 \\
\bar{P}_{2NI} & 0.27 & 0.43 & 0.39 & 0.35 \\
\Delta S_{NI} & 0.07 & 0.55 & 0.33 & \\
t^* & \sim 0.002 & 0.092 & 0.054 & 0.038 \\
\end{array}
\]

\(^a\) Luckhurst and Simpson 1982, \(^b\) Sheng and Wojtowicz (1976), \(^c\) Van der Haegh \textit{et al} (1980).
The model has proved to correctly account for the essential symmetry of liquid crystalline orientational order and has been generalized to more complex situations.

(a) $(P_L, P_M)$ models: $(L,M) = (2,4), (2,1)$

(b) investigation of the nematic ordering in confined geometries, subject to different surface anchoring fields (grating, patterned surfaces, ...),

(c) effect of an external field on the isotropic - nematic phase transition(s),

(d) simulations of electro-optical devices,

(e) simulation of chiral liquid crystal phases,

(f) orientational properties of polymers and elastomers and

(g) physics of two-dimensional systems (no topological phase transitions in $O(3)$ symmetric two dimensional (LL-molecules can reorient in three dimensions))

1. Lattice models emphasize symmetry aspects of orientational order
2. Discretized versions of Landau-deGennes theories $\Rightarrow$ LL models
3. The same form of „effective” interaction for hard bodies (Onsager) and dispersion interactions ($t \leftrightarrow 1/\rho$)
Outline


2. Spontaneously generated chiral states in the presence of quadrupolar and octupolar interactions.

3. Possibility of phases with splay-twist-bent deformations.

4. Summary

Wikipedia 'Thermodynamics'

Three Laws of Thermodynamics:
1. You can't win.
2. You can't break even.
3. You can't even quit the game.
Interacting biaxial quadrupoles of $D_{2h}$ symmetry:

$$V = \sum_{\alpha, \beta=1}^{3} \bar{\omega}_{\alpha\beta} (b_\alpha \cdot l_\beta)^2$$

$\bar{\omega}_{\alpha\beta} = \bar{\omega}_{\beta\alpha}$ symmetry interchange of $l$ and $b$ vectors

6 parameters! (too many)
Interacting biaxial quadrupoles of $D_{2h}$ symmetry

\[ Q_{U,b} \equiv T_0^2(\Omega_b) = \sqrt{\frac{3}{2}} \left( b_3 \otimes b_3 - \frac{1}{3} I \right) \]

\[ Q_{B,b} \equiv T_2^2(\Omega_b) = \frac{1}{\sqrt{2}} \left( b_1 \otimes b_1 - b_2 \otimes b_2 \right) \]

\[ T_m^L \cdot T_{m'}^{L'} = (T_m^L)_{\alpha \beta} \cdots (T_{m'}^{L'})_{\alpha \beta} \cdots = \delta_{mm'} \delta_{LL'} \]
Interacting biaxial quadrupoles of $D_{2h}$ symmetry: (3d cubic lattice, nearest-neighbour interactions)

\[ V = \overline{w}_{2,00} Q_{U,b} \cdot Q_{U,1} + \overline{w}_{2,20} [Q_{U,b} \cdot Q_{B,1} + Q_{B,b} \cdot Q_{U,1}] + \overline{w}_{2,22} Q_{B,b} \cdot Q_{B,1} \]

\[ = \left( \overline{w}_{2,22} - \sqrt{3} \overline{w}_{2,20} \right) (b_1 \cdot l_1)^2 + \left( \overline{w}_{2,22} + \sqrt{3} \overline{w}_{2,20} \right) (b_2 \cdot l_2)^2 + \]

\[ \left( \frac{3}{2} \overline{w}_{2,00} - \frac{\overline{w}_{2,22}}{2} \right) (b_3 \cdot l_3)^2 + \text{const} \]

\[ F = -k_B T \ln(Z); \quad Z = Tr_{\{\Omega_1, \ldots, \Omega_N\}} e^{-\beta V} \]
Duality transformation

\[ F = -k_B T \ln(Z); \quad Z = \text{Tr}_{\{\Omega_1, \ldots, \Omega_N\}} e^{-\beta V_N} \]

\[ \beta V = \beta \left[ \left( \overline{w}_{2,22} - \sqrt{3} \overline{w}_{2,20} \right) (b_1 \cdot l_1)^2 + \left( \overline{w}_{2,22} + \sqrt{3} \overline{w}_{2,20} \right) (b_2 \cdot l_2)^2 + \left( \frac{3}{2} \overline{w}_{2,00} - \frac{\overline{w}_{2,22}}{2} \right) (b_3 \cdot l_3)^2 \right] \]

\[ = -v_{00} \left[ \left( v_2 - \sqrt{3} v_0 \right) (b_1 \cdot l_1)^2 + \left( v_2 + \sqrt{3} v_0 \right) (b_2 \cdot l_2)^2 + \left( \frac{3}{2} \text{sign}(v_{00}) - \frac{v_2}{2} \right) (b_3 \cdot l_3)^2 \right] \]

\[ \text{sign}(v_{00}) = 1 \]

\[ \beta |\overline{w}_{2,00}| = |v_{00}| = 1/t \]
\[ \beta V = -\frac{1}{t} \left[ \left( v_2 - \sqrt{3} v_0 \right) (b_1 \cdot l_1)^2 + \left( v_2 + \sqrt{3} v_0 \right) (b_2 \cdot l_2)^2 + \left( \frac{3}{2} \text{sign}(v_{00}) - \frac{v_2}{2} \right) (b_3 \cdot l_3)^2 \right] \]

Complete bifurcation diagram for $\text{sign}(v_{00}) > 0$. The upper surface, tailed by larger squares, represents bifurcation from the isotropic phase. The second surface gives the bifurcation temperature from uniaxial to biaxial states. Tricritical temperatures are marked with continuous, black line.
\[ \beta V = \beta \left[ \left( \bar{w}_{2,22} - \sqrt{3} \bar{w}_{2,20} \right) (b_1 \cdot l_1)^2 + \left( \bar{w}_{2,22} + \sqrt{3} \bar{w}_{2,20} \right) (b_2 \cdot l_2)^2 + \left( \frac{3}{2} \bar{w}_{2,00} - \frac{\bar{w}_{2,22}}{2} \right) (b_3 \cdot l_3)^2 \right] \]

<table>
<thead>
<tr>
<th>Models</th>
<th>( \bar{w}_{2,00} )</th>
<th>( \bar{w}_{2,20} )</th>
<th>( \bar{w}_{2,22} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Straley [5]</td>
<td>( \beta )</td>
<td>( \frac{2}{\sqrt{3}} \gamma )</td>
<td>( \delta )</td>
</tr>
<tr>
<td>Dispersion model [16–20]</td>
<td>(-\epsilon)</td>
<td>( \sqrt{2} \epsilon \lambda )</td>
<td>(-2\epsilon \lambda^2)</td>
</tr>
<tr>
<td>Two-tensor [12]</td>
<td>(-\frac{2V_0}{3})</td>
<td>(-\frac{2\sqrt{3}}{3} V_0 \gamma)</td>
<td>(-2V_0 \lambda)</td>
</tr>
</tbody>
</table>

\[ \tilde{W}_{2,00} = -\varepsilon \]
\[ \tilde{W}_{2,20} = \sqrt{2}\varepsilon \lambda \]
\[ \tilde{W}_{2,22} = -2\varepsilon \lambda^2 \]

Geometric mean rule for interactions (Berthelot rule)

\[ \tilde{V}(i, j) = -\varepsilon \mathbf{Q}(i) \cdot \mathbf{Q}(j) \]

\[ Q = \left( \hat{T}_0^{(2)}(\Omega_i) + \sqrt{2} \lambda \hat{T}_2^{(2)}(\Omega_i) \right) \]

Molecular polarizibility tensor

Uniaxial tensor

Biaxial tensor

Geometric mean rule for interactions (Berthelot rule)

\[ \lambda = \sqrt{\frac{3}{2}} \frac{\alpha_{xx} - \alpha_{yy}}{2\alpha_{zz} - (\alpha_{xx} + \alpha_{yy})} \]
\[ \varepsilon = (2\alpha_{zz} - (\alpha_{xx} + \alpha_{yy}))^2. \]
Outline


2. Spontaneously generated chiral states in the presence of quadrupolar and octupolar interactions.


4. Summary
Chirality

handedness, from the Greek χειρ

The word 'chiral', meaning handed, was first introduced into science by Lord Kelvin (William Thomson), Professor of Natural Philosophy in the University of Glasgow from 1846-1899:

I call any geometrical figure, or group of points, chiral, and say that it has chirality, if its image in a plane mirror, ideally realized, cannot be brought to coincide with itself.

Lord Kelvin, Baltimore Lectures, 1884
Chiral interactions:

Measure of chirality

$K$
Chirality breaking from non-chiral molecules

Reviews:

Vol. 45, No. 2A, 2006, pp. 597–625


- Spontaneous chiral deracemization at microscopic and macroscopic levels occurs and is controllable (banana smectic ph.)

- achiral bent-core molecules enhance system chirality
- polarizers under decrossed conditions - method of confirming chiral segregated domains

• Chiral symmetry breaking also has been reported in the nematic phase of achiral fluid bent-core liquid crystals:


analyser rotated clockwise and anticlockwise by the same angle

• Selfassembly of twisted conformers
• Conical twist-bend deformations

Dimensionless deGennes - Ginzburg - Landau:

\[ F = \int_V \left\{ \frac{1}{2} a \text{Tr} (Q^2) - \text{Tr} (Q^3) + [\text{Tr} (Q^2)]^2 + \cdots + (\nabla \otimes Q)^2 + \rho (\nabla \cdot Q)^2 + \cdots \right\} \]

\[ S^2 + T^2 + B^2 \]

\[ S^2 + B^2 \]

\[ \rho > -\frac{2}{3} \]

Oseen-Zocher-Frank:

\[ Q = S \left( n \otimes n - \frac{1}{3} \mathbf{1} \right) \]

\[ F = \frac{1}{2} \int_V \left[ K_1 (\nabla \cdot n)^2 + K_2 (n \cdot \nabla \times n)^2 + K_3 (n \times \nabla \times n)^2 \right] \]
Chirality: phenomenological level  (orientational order only)  
(Dimensionless) minimal coupling  
Landau-deGennes free energy

\[ F = \int \left\{ \frac{1}{2} \alpha \text{Tr} \left( Q^2 \right) - \text{Tr} \left( Q^3 \right) + \left[ \text{Tr} \left( Q^2 \right) \right]^2 + \cdots + \left( \nabla \otimes Q \right)^2 + \rho \left( \nabla \cdot Q \right)^2 - 2\kappa \epsilon_{\alpha \beta \gamma} Q_{\alpha \mu} \partial_\beta Q_{\gamma \mu} \right\} \]

Splay, twist, bend  … deformations are weighted by these terms
CALCULATIONS IN FOURIER SPACE:

\[ Q(\mathbf{r}) = \sum_{\mathbf{k}} \sum_{m=-2}^{2} \mu_m(\mathbf{k}) M_m(\mathbf{\hat{k}}) e^{i\mathbf{k} \cdot \mathbf{r}} \]

\[ e_{0,\mathbf{k}}^{[2]} = \frac{1}{\sqrt{6}} \left\{ 3\mathbf{\hat{k}} \otimes \mathbf{\hat{k}} - 1 \right\}, \]
\[ e_{\pm 1,\mathbf{k}}^{[2]} = \pm \frac{1}{2} \left\{ (\mathbf{\hat{v}} \pm i\mathbf{\hat{w}}) \otimes \mathbf{\hat{k}} + \mathbf{\hat{k}} \otimes (\mathbf{\hat{v}} \pm i\mathbf{\hat{w}}) \right\}, \]
\[ e_{\pm 2,\mathbf{k}}^{[2]} = \frac{1}{2} \left\{ (\mathbf{\hat{v}} \pm i\mathbf{\hat{w}}) \otimes (\mathbf{\hat{v}} \pm i\mathbf{\hat{w}}) \right\} \]

\[ M_m(\mathbf{\hat{k}}) \cdot M_{m'}^{*}(\mathbf{\hat{k}}) \equiv \text{Tr} \left( M_m(\mathbf{\hat{k}}) M_{m'}^{*}(\mathbf{\hat{k}}) \right) = \delta_{mm'} \]

\[ e_{m,\mathbf{k}}^{[2]} \equiv M_m(\mathbf{\hat{k}}) \]
\[ F = \int \nu \left\{ \frac{1}{2} a \text{Tr} (Q^2) - \text{Tr} (Q^3) + \left[ \text{Tr} (Q^2) \right]^2 + \cdots \right\} \]

\[ + (\nabla \otimes Q)^2 + \rho (\nabla \cdot Q)^2 \]

\[ - 2\kappa \epsilon_{\alpha\beta\gamma} Q_{\alpha\mu} \partial_{\beta} Q_{\gamma\mu} \}

\[ F_2 = \frac{1}{4} \sum_k \sum_m \left\{ t - m \kappa k + \left[ 1 + \frac{1}{6} \rho (4 - m^2) \right] k^2 \right\} |\mu_m(k)|^2 \]

\[ t = a = a_0 (T - T^*) \]

Cholesteric phase
Chirality: phenomenological level (orientational order only)  
(Dimensionless) Landau-deGennes free energy

\[
F = \int \left\{ \frac{1}{2} \alpha \text{Tr} \left( Q^2 \right) - \text{Tr} \left( Q^3 \right) + \left[ \text{Tr} \left( Q^2 \right) \right]^2 + \cdots 
+ \left( \nabla \otimes Q \right)^2 + \rho \left( \nabla \cdot Q \right)^2 - 2\kappa \epsilon_{\alpha\beta\gamma} Q_{\alpha\mu} \partial_\beta Q_{\gamma\mu} \right\}
\]

Where does the totally antisymmetric tensor come from?

- for ordinary chiral materials:

tetrahedrally coordinated molecule

B. Harris, R. D. Kamien, and T. C. Lubensky, RMP, Vol. 71, 1999
Chirality: phenomenological level (orientational order only)

(Dimensionless) Landau-deGennes free energy

$$F = \int \left\{ \frac{1}{2} a \text{Tr} \left( Q^2 \right) - \text{Tr} \left( Q^3 \right) + \left[ \text{Tr} \left( Q^2 \right) \right]^2 + \cdots + \left( \nabla \otimes Q \right)^2 + \rho \left( \nabla \cdot Q \right)^2 - 2 \kappa \epsilon_{\alpha\beta\gamma} Q_{\alpha\mu} \partial_\beta Q_{\gamma\mu} \right\}$$

For nonchiral molecules:

where does the totally antisymmetric tensor come from?
From symmetry point of view there are 2 possibilities that can be read from the previous Landau-deGennes formula:

\[ + (\nabla \otimes \mathbf{Q})^2 + \rho (\nabla \cdot \mathbf{Q})^2 \]

should be replaced by:

\[ (\partial_\alpha Q_\beta \gamma - u T_{\alpha \beta \gamma})^2 \quad \text{and/or} \quad (\partial_\alpha Q_\alpha \gamma - u P_\gamma)^2 \]

octupolar tensor \quad \text{Polar vector}

and lowest order bulk chiral invs.

\[ \epsilon_{\alpha \beta \gamma}(Q^2)_{\alpha \delta} Q_{\beta \varepsilon} T_{\delta \varepsilon \gamma} \cdot P_\alpha P_\beta P_\gamma \varepsilon_{\alpha \mu \nu} Q_{\mu \beta} Q^{2}_{\nu \gamma} \]

\[ \epsilon \sim Q^2 QT \sim PPPQQQ^2 \]
Partial discussion of these issues can be found in (work is still in progress):

Spontaneous polarization in chiral biaxial liquid crystals
Lech Longa and Hans-Rainer Trebin

Theory of bent-core liquid-crystal phases and phase transitions
T. C. Lubensky
Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19174
Leo Radzihovsky
Department of Physics, University of Colorado, Boulder, Colorado 80309

Chiral symmetry breaking in bent-core liquid crystals
Lech Longa,1,* Grzegorz Pająk,1 and Thomas Wydro1,2,†

Tetrahedral mesophases, chiral order, and helical domains induced by quadrupolar and octupolar interactions
Karol Trojanowski,1 Grzegorz Pająk,1,2 Lech Longa,1,* and Thomas Wydro1,3,†
Mass distribution:

The ‘steric dipole’ mass moment

\[ C_{1,\alpha}^i = \sum_{\mu=1}^{3} m_\mu r_{\alpha,\mu}^2 r_{\alpha,\mu}^i \]

The second mass moment

\[ C_{2,\alpha}^{ij} = \sum_{\mu=1}^{3} m_\mu \left( r_{\alpha,\mu}^i r_{\alpha,\mu}^j - \frac{1}{3} r_{\alpha,\mu}^2 \delta^{ij} \right) \]

The third mass moment

\[ C_{3,\alpha}^{ijk} = \sum_{\mu=1}^{3} m_\mu \left[ r_{\alpha,\mu}^i r_{\alpha,\mu}^j r_{\alpha,\mu}^k - \frac{1}{3} r_{\alpha,\mu}^2 \left( \delta^{ij} r_{\alpha,\mu}^k + \delta^{ik} r_{\alpha,\mu}^j + \delta^{jk} r_{\alpha,\mu}^i \right) \right] \]

Dipole, quadrupole and octupole order parameters are relevant for bent-core systems

These 2 tensors are needed to get chiral order

Chirality is a combined effect of biaxial-quadrupolar and octupolar (local or global) order

\[ \Xi_{ijk} = Q^{is} B^{jt} T^{stk} + Q^{js} B^{kt} T^{sti} + Q^{ks} B^{it} T^{stj} \]

\[ \Xi_{ijk} Q^{il} \nabla_j Q^{kl} \]
Generic Lebwohl Lasher lattice model:
- quadrupoles and octupoles occupy lattice sites,
- dipoles are disregarded
- cross-coupling terms involve $Q$ and $T$ and $r$
- two-fold axes of the tensors coincide

$$Q = (Q_U + \sqrt{2} \lambda Q_B)$$

$$V(i, j) \approx -\varepsilon \left( Q(i) \cdot Q(j) + \tau T(i) \cdot T(j) \right)$$

+ c.c.t $(Q,T,r)$

Degrees of freedom: proper rotations + parity: $p_k = \hat{a}_k \cdot (\hat{b}_k \times \hat{c}_k) = \pm 1$
**Order parameters**

\[ Q_U \equiv T_0^{(2)} = \frac{3}{2} \left( \hat{c}_k \otimes \hat{c}_k - \frac{1}{3} \mathbf{1} \right) \]

\[ Q_B \equiv T_2^{(2)} = \frac{1}{2} \left( \hat{a}_k \otimes \hat{a}_k - \hat{b}_k \otimes \hat{b}_k \right) \]

\[ T \equiv T_2^{(3)} = \frac{1}{\sqrt{6}} \sum_{(\hat{x}, \hat{y}, \hat{z}) \in \pi \left( \hat{a}_k, \hat{b}_k, \hat{c}_k \right)} \hat{x} \otimes \hat{y} \otimes \hat{z} \]

parity \( p_k = \hat{a}_k \cdot \left( \hat{b}_k \times \hat{c}_k \right) = \pm 1 \)

\[
\text{Tr}_{(1,\ldots,N)} \equiv \prod_{k=1}^{N} \left( \frac{1}{2} \sum_{p_k=\pm 1} \int \! d\Omega' \right)
\]

\[ F = -k_B T \ln(Z); \quad Z = \text{Tr}_{\{p_1 \Omega_1, \ldots, p_N \Omega_N\}} e^{-\beta V_N} \]

L. Longa, G. Pająk, and T. Wydro, PRE 79, 040701R 2009
\[ V(i, j) \approx -\varepsilon (Q(i) \cdot Q(j) + \tau T(i) \cdot T(j)) \]

\[ Q = (Q_u + \sqrt{2} \lambda Q_n) \]

\[ \tau = 1. \]

\[ \bar{p} \approx \frac{\sqrt{2}}{210t^4} \tau \lambda (-3 + 2\lambda^2) \Delta_{22}^{(3)} \left( \Delta_{20}^{(2)} + \sqrt{2}\lambda \Delta_{22}^{(2)} \right)^3 \]
\[ V(i, j) \approx -\varepsilon \left( \mathbf{Q}(i) \cdot \mathbf{Q}(j) + \tau \mathbf{T}(i) \cdot \mathbf{T}(j) \right) \]

\[ \mathbf{Q} = (\mathbf{Q}_U + \sqrt{2} \lambda \mathbf{Q}_B) \]

\[ \tau = 9 \]

Isotropic: \( I \{ O(3) \} \)

Uniaxial: \( N_U \{ D_{\infty h} \} \)

\( \Delta^{(2)}_{22} \)

\( \Delta^{(3)}_{22} \)

Tetrahedral: \( T \{ T_d \} \)

\( \Delta^{(2)}_{00} \)

\( \Delta^{(3)}_{22} \)

Biaxial: \( N_B \{ D_{2h} \} \)

\( \Delta^{(3)}_{22} \)

\( \Delta^{(2)}_{22} \)

Nematic

\( \Delta^{(2)}_{00} \)

\( \Delta^{(3)}_{22} \)

Tetrahedral: \( N_T \{ D_{2d} \} \)

Chiral: \( N_T^* \{ D_2 \} \)

\[ \bar{p} \approx \frac{\sqrt{2}}{210t^4} \lambda \tau \left( -3 + 2\lambda^2 \right) \Delta^{(3)}_{22} \left( \Delta^{(2)}_{20} + \sqrt{2}\lambda \Delta^{(2)}_{22} \right)^3 \]
Observation of a possible tetrahedral phase in a bent-core liquid crystal

D. Wiant, K. Neupane, S. Sharma, J. T. Gleeson, and S. Sprunt
Department of Physics Kent State University, Kent, Ohio 44242, USA

A. Jákli
Chemical Physics Interdisciplinary Program and Liquid Crystal Institute,
Kent State University, Kent, Ohio 44242, USA

N. Pradhan and G. Iannacchione

DOI: 10.1002/ptr.20110101

Tetrahedral Mesophases, Ambidextrous Chiral Domains and Helical Superstructures Produced by Achiral 1,1′-Disubstituted Ferrocene Derivatives

Eun Ho Kim,[a] Oleg Nikolaevich Kadkin,[a,b] So Yeon Kim,[a] and Moon-Gun Choi*[a]


Figure 4. Molecular models of tetrahedral associates in 1a and mirror relationships in the bent conformers.
\[ V(i, j) \approx -\epsilon \left( Q(i) \cdot Q(j) + \tau T(i) \cdot T(j) \right) \]

\[ V_c(p_i, \Omega'_i, p_j, \Omega'_j) \]
\[ = \frac{\kappa}{\epsilon} \left[ b_{\alpha i} \cdot (b_{\beta i} \times b_{\gamma i}) Q_{\alpha v}(\Omega_i) Q_{\beta v}(\Omega_j) 
- b_{\alpha j} \cdot (b_{\beta j} \times b_{\gamma j}) Q_{\alpha v}(\Omega_j) Q_{\beta v}(\Omega_i) \right] (\hat{r}_{ij})^\gamma \]

\[ b_{\alpha} \cdot (b_{\beta} \times b_{\gamma}) = 2\sqrt{2} \sum_{(x,y,z) \in c\{\alpha,\beta,\gamma\}} T_{0,x\mu}^2 T_{2,yv}^2 T_{2,\mu vz}^3, \]

summation runs over cyclic permutations of \(\{\alpha, \beta, \gamma\}\)
\(c\{\alpha, \beta, \gamma\} = \{(\alpha, \beta, \gamma), (\gamma, \alpha, \beta), (\beta, \gamma, \alpha)\}\).
$\lambda = 0.3, \quad \tau = 1$
\( \lambda = 0.3, \quad \tau = 1, \quad \kappa = 1 \)

t=0.2
\[ \lambda = 0.3, \quad \tau = 1, \quad \kappa = \]

\[ t = 0.55 \]
\[
\lambda = 0.3, \quad \tau = 1, \quad \kappa = 1
\]

t=0.55
\[ \lambda = 0.3, \quad \tau = 1, \quad \kappa = 1 \]

t = 0.7
$\lambda = 0.3, \quad \tau = 1, \quad \kappa = 1$
Outline


2. Spontaneously generated chiral states in the presence of quadrupolar and octupolar interactions.


4. Summary
A discussed previously:

\[ + (\nabla \otimes \mathbf{Q})^2 + \rho (\nabla \cdot \mathbf{Q})^2 \]

should be replaced by:

\[
(\partial_{\alpha} Q_{\beta\gamma} - u T_{\alpha\beta\gamma})^2 \quad \text{and/or} \quad (\partial_{\alpha} Q_{\alpha\gamma} - u P_{\gamma})^2
\]

- octupolar tensor
- Polar vector

Ground state deformations should contain all possible modes as discussed on p. 22. In addition: (a) presence of T or P fields renormalizes elastic constants of nematics; (b) coupling of Q with P can stabilize helical polar structures; (c) presence of T tensor can give interesting optical properties of the system.
Summary:

• The simplest model with quadrupolar and octupolar interactions gives 3 new structures; one of them is chiral.

• Cross-coupling terms impose spatially modulated order.

• Different scenarios are possible when twofold axes of Q and T tensors do not coincide ($D_{3h} - symmetric$ str.).

• Polar order (dipole-dipole int.) and various scenarios of Q, T and P couplings are subject to present studies.
Thank you for your attention.