The handle http://hdl.handle.net/1887/42793 holds various files of this Leiden University dissertation.

**Author:** Liu, K.
**Title:** Gauge theory and nematic order : the rich landscape of orientational phase transition
**Issue Date:** 2016-09-06
Chapter 5

Generalized biaxial phase transitions

“Vestigial” or “mesophases” of matter are a well established part of the canon of spontaneous symmetry breaking. It might well happen that due to thermal [11] (or even quantum [12]) fluctuations a phase is stabilized at intermediate temperatures (or coupling constant at $T = 0$) characterized by a symmetry intermediate between the high temperature isotropic phase and the fully symmetry broken phase at low temperature (small coupling constant). Iconic examples are liquid crystals [11], occurring in between the high temperature liquids and the low temperature crystals, characterized by only the breaking of the rotational symmetry (“nematics”), followed potentially by a partial breaking of translations (“smectic” or “columnar” phases) before full solidification sets in.

In the general sense of phases of matter that break the isotropy of Euclidean three dimensional space, nematic liquid crystals are in principle classified in terms of all subgroups of $O(3)$: the family of three dimensional point groups. There are a total of seven infinite axial families and seven polyhedral groups of such symmetries, exhibiting a very rich subgroup hierarchy. Accordingly, in principle it is allowed by symmetry to realize a very rich hierarchy of rotational vestigial phases, where upon lowering temperature phases in this symmetry hierarchy would be realized one after the other.

In experimental reality this is not encountered. Nearly all of the vast empirical landscape of liquid crystals deals with one particular form of nematic order: the uniaxial nematic characterized by the $D_{\infty h}$ point-group with “rod-like” molecules or mesogens that line up in the nematic phase. Another well established form is the “biaxial nematic” formed from platelets with three inequivalent director axes, characterized by the $D_{2h}$ point group symmetry [72, 74, 67, 70, 69, 98, 99, 71]. $D_{2h}$ is a subgroup of $D_{\infty h}$ and it is well understood that the uniaxial nematic can be
a vestigial mesophase that can occur in between the isotropic and biaxial phase. In order for such vestigial rotational sequences to occur special microscopic conditions are required: dealing with molecule-like mesogenic constituents, special anisotropic interactions have to be present.

We will discuss in this chapter, the symmetry structure and anisotropic interactions that are behind the $D_{2h}$ uniaxial-biaxial phase descendence are actually perfectly compatible with all axial groups. As a consequence, the generalization of the special uniaxial-biaxial type of vestigial symmetry lowering is possible for this vast number of symmetries. Particularly, the gauge theory we introduced in Chapter 3 allows one to incorporate these generalized biaxial transitions in a natural and efficient manner.

5.1 The structure of nematic order parameters and generalized biaxial transitions

Three dimensional generalized nematics break the rotational group $O(3)$ down to a three-dimensional point group. By the Landau-de Gennes symmetry paradigm, phase transitions between any two nematic phases related by the subgroup structure of $O(3)$ are allowed, apart from transitions between the isotropic $O(3)$ phase and a generalized nematic phase. In this section, we will show that the order parameter structure of axial nematics provides a natural way to realize some of these allowed transitions. We then discuss how to realize these phase transitions by tuning the couplings in our lattice model in Section 5.2.

5.1.1 Point groups and nematic order parameters

Three-dimensional point groups are classified in terms of seven finite polyhedral groups, \{$T, T_d, T_h, O, O_h, I, I_h$\}, and seven infinite families of axial groups, \{$C_n, C_{nv}, S_{2n}, C_{nh}, D_n, D_{nh}, D_{nd}$\} \cite{131, 95}. The associated nematic order parameters are tensors that are invariant under the given point-group symmetry. We have discussed these order parameters and their derivation in Chapter 4. Now we review the results that are needed in the following.

Three dimensional orientation can be parametrized in terms of a $O(3)$ matrix

$$R = \left(1 \quad \mathbf{m} \quad \mathbf{n}\right)^T.$$  (5.1)
The rows \( \mathbf{n}^\alpha = \{\mathbf{l}, \mathbf{m}, \mathbf{n}\} \) of \( R \) form an orthonormal triad and satisfy the additional \( O(3) \) constraint

\[
\sigma = \det R = \epsilon_{abc} (\mathbf{l} \otimes \mathbf{m} \otimes \mathbf{n})_{abc} = \mathbf{l} \cdot (\mathbf{m} \times \mathbf{n}) = \pm 1, \tag{5.2}
\]

where \( \sigma \) is the chirality or handedness of the triad \( \mathbf{n}^\alpha \) associated with \( R \).

The order parameter tensors are constructed from tensor products of \( R \) and we use the point group conventions as those in Chapter 4. In case of the polyhedral nematics \( G = \{T, T_d, T_h, O, O_h, I, I_h\} \), the general form of the order parameter is given by \( O^G = \{O^G[\mathbf{l} \; \mathbf{m} \; \mathbf{n}], \sigma\} \), where \( O^G[\mathbf{l} \; \mathbf{m} \; \mathbf{n}] \) describes the orientational order of the phase and \( \sigma \) is a chiral order parameter needed for the proper polyhedral groups \( \{T, O, I\} \). The polyhedral groups have several higher order rotation axes and transform the triads \( \{\mathbf{l}, \mathbf{m}, \mathbf{n}\} \) irreducibly: in these cases we only need one tensor to describe the orientational order.

On the other hand, the axial groups \( \{C_n, C_{nv}, S_{2n}, C_{nh}, D_n, D_{nh}, D_{nd}\} \) are defined with respect to a symmetry plane involving rotations and/or reflections as well as a perpendicular, axial direction. Correspondingly, the order parameter tensors of the axial point groups have the general structure \( O^G = \{A^G, B^G, \sigma\} \), where \( A^G \) defines the ordering related to the orientation of the so-called primary axis perpendicular to the symmetry plane and \( B^G \) describes the in-plane ordering. We refer to \( A \) as the axial order and \( B \) as the in-plane (or just biaxial) order \cite{32}. Similarly, \( \sigma \) is the chiral ordering for the proper axial groups \( \{C_n, D_n\} \). Note that the \( O(3) \) constraints can reduce the number of independent order parameter tensors in the set \( \{A^G, B^G, \sigma\} \). Following the conventions in Chapter 4, \( \mathbf{n} \) is chosen always to be along the primary axis. Then the axial order parameter tensor \( A^G = A^G[\mathbf{n}] \) depends only on \( \mathbf{n} \) by construction. It follows that the axial order parameter tensor \( A^G = A^G[\mathbf{n}] \) depends only on \( \mathbf{n} \) by construction. Similarly, the in-plane order parameter \( B^G = B^G[\mathbf{l}, \mathbf{m}] \) depends only on \( \{\mathbf{l}, \mathbf{m}\} \) for the symmetries \( G = \{C_n, C_{nv}, C_{nh}, D_n, D_{nh}\} \), but is a tensor polynomial \( B^G = B^G[\mathbf{l}, \mathbf{m}, \mathbf{n}] \) of all the three triads for the symmetries \( \{S_{2n}, D_{nd}\} \). We have discussed these ordering tensors in Chapter 4, but for the convenience of the readers, in Table 5.1 we show a selection of axial nematic ordering tensors for the groups which are later encountered.

Moreover, because of the common structure of the axial point groups, the tensors \( A^G \) and \( B^G \) are not unique to a given symmetry, though the axial point group ordering can be uniquely defined by the full set of order
parameters \{A^G, B^G, \sigma\}. For instance, the symmetry groups \(C_n\) and \(C_{nv}\) do not transform the primary axis \(n\), thus the axial ordering tensor for symmetries in these types is simply a vector,

\[
A^{C_n}[n] = A^{C_{nv}}[n] = A^{C_{\infty v}}[n] = n,
\]

which is just the well-known director order parameter for \(D_{\infty h}\)-uniaxial nematics. Note that \(D_{\infty h}\) can be considered as the continuous limit of the finite groups \(D_{nh}\) and \(D_{nd}\), whereas \(C_{\infty h}\) arises from the limit of \(C_{nh}\) and \(S_{2n}\). Similarly, axial nematics with the same \(n\)-fold in-plane symmetries have the same ordering tensor \(B\),

\[
B^{C_n}[l, m] = B^{C_{nh}}[l, m],
\]

\[
B^{C_{nv}}[l, m] = B^{D_n}[l, m] = B^{D_{nh}}[l, m].
\]

Note that, however, though the axial and the biaxial ordering tensors are distinct and transform irreducibly, they are not completely independent due to the \(O(3)\) constraints of orthonormality and Eq. (5.2).

### 5.1.2 Generalized biaxial phases and transitions

The distinction between the primary axis \(n\) and the in-plane axes \(l\) and \(m\) for axial nematics allows the disordering of the axial and in-plane order separately.

A familiar example is the biaxial-uniaxial-isotropic liquid transitions of \(D_{2h}\)-biaxial liquid crystals [72–75, 86, 93]. The order parameter tensors of the \(D_{2h}\) nematic are defined by two linearly independent rank-2 tensors, \(O^{D_{2h}} = \{A^{D_{2h}}[n], B^{D_{2h}}[l, m]\}\), where \(A^{D_{2h}}[n]\) has been give in Eq. (5.4), and \(B^{D_{2h}}[l, m]\) is the well-known biaxial order parameter,

\[
B^{D_{2h}}[l, m] = l \otimes l - m \otimes m.
\]
Table 5.1. A selection of three-dimensional nematic order parameters.
The first column specifies the symmetries, the second column specifies the type
\{A, B\} of the order, and the third column gives the explicit form of ordering
tensors. Besides the tensor shown here, chial nematics \(C_2\) and \(D_2\) in addition
have a chiral order parameter defined by \(\sigma\).

<table>
<thead>
<tr>
<th>Symmetry Groups</th>
<th>Type</th>
<th>Ordering Tensors</th>
</tr>
</thead>
<tbody>
<tr>
<td>(S_2)</td>
<td>(B[l, m, n])</td>
<td>(l \otimes m, m \otimes n, n \otimes l)</td>
</tr>
<tr>
<td>(C_2, C_{2h})</td>
<td>(B[l, m])</td>
<td>(l \otimes m)</td>
</tr>
<tr>
<td>(C_{2v}, D_2, D_{2h})</td>
<td>(B[l, m])</td>
<td>(1 \otimes 1 - \frac{1}{3}I, m \otimes m - \frac{1}{3}I)</td>
</tr>
<tr>
<td>(S_4)</td>
<td>(B[l, m, n])</td>
<td>((1 \otimes 1 - m \otimes m) \otimes n)</td>
</tr>
<tr>
<td>(D_{2d})</td>
<td>(B[l, m, n])</td>
<td>((1 \otimes m + m \otimes 1) \otimes n)</td>
</tr>
<tr>
<td>(C_2, C_{2v}, C_{\infty})</td>
<td>(A[n])</td>
<td>(n)</td>
</tr>
<tr>
<td>(S_2, C_{2h}, D_2, D_{2h}, D_{2d}, D_{\infty})</td>
<td>(A[n])</td>
<td>(n \otimes n - \frac{1}{3}I)</td>
</tr>
</tbody>
</table>

In terms of the symmetries, the biaxial nematic order allows for the phase transitions

\[D_{2h} \rightarrow D_{\infty h} \rightarrow O(3),\]

upon increasing temperature. That is, upon increasing temperature, the
biaxial order is destroyed first leading to the restoration of the in-plane
\(O(2)\) symmetry of uniaxial nematics before the transition to the fully
disordered isotropic phase takes place.

Given the general order parameter structure of axial nematics dis-
cussed in Section 5.1.1, this transition sequence can be directly generalized
to other axial symmetries. We will refer to the associated phase transi-
tions as generalized biaxial transitions. Namely, by first destroying the
in-plane order \(B\), the following generalized biaxial-uniaxial transition can be induced

\[C_n, C_{nv} \rightarrow C_{\infty v},\]
\[S_{2n}, C_{nh}, D_n, D_{nh}, D_{nd} \rightarrow D_{\infty h}.\]
Table 5.2. Generalized biaxial phase transitions. The first column specifies the generalized nematic symmetries and the second column the minimal set of order parameter tensors. Relations of the order parameters given by Eqs. (5.3)–(5.5) are indicated. For the explicit form of these order parameters see Table 4.1. The third and fourth column show the order parameter tensors involved in the generalized biaxial-uniaxial transitions in Eq. (5.8) and the biaxial-biaxial transitions in Eq. (5.11), respectively. The symbol “→” indicates the replacement of an order.

<table>
<thead>
<tr>
<th>Symmetry</th>
<th>Order Parameters</th>
<th>Uniaxial-biaxial Transitions</th>
<th>Biaxial-biaxial* (Uniaxial-uniaxial*) Transitions</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_n$</td>
<td>$A^{C_n} = A^{C_{\infty}}[n]$, $B^{C_n} = B^{C_{nh}}[l,m], \sigma$</td>
<td>$B^{C_{nh}}[l,m], \sigma$</td>
<td>$A^{C_{\infty}}[n] \rightarrow A^{D_{\infty}}[n], \sigma$</td>
</tr>
<tr>
<td>$C_{nv}$</td>
<td>$A^{C_{nv}} = A^{C_{\infty}}[n]$, $B^{C_{nv}} = B^{D_{nh}}[l,m]$</td>
<td>$B^{D_{nh}}[l,m]$</td>
<td>$A^{C_{\infty}}[n] \rightarrow A^{D_{\infty}}[n]$</td>
</tr>
<tr>
<td>$S_{2n}$</td>
<td>$A^{S_{2n}} = A^{D_{nh}}[n]$, $B^{S_{2n}}[l,m,n]$</td>
<td>$B^{S_{2n}}[l,m,n] \rightarrow B^{C_{2nh}}[l,m]$</td>
<td></td>
</tr>
<tr>
<td>$C_{nh}$</td>
<td>$A^{C_{nh}} = A^{D_{nh}}[n]$, $B^{C_{nh}}[l,m]$</td>
<td>$B^{C_{nh}}[l,m]$</td>
<td>None</td>
</tr>
<tr>
<td>$D_n$</td>
<td>$A^{D_n} = A^{D_{nh}}[n]$, $B^{D_{nh}}[l,m], \sigma$</td>
<td>$B^{D_{nh}}[l,m], \sigma$</td>
<td>$\sigma$</td>
</tr>
<tr>
<td>$D_{nh}$</td>
<td>$A^{D_{nh}} = A^{D_{nh}}[n]$, $B^{D_{nh}}[l,m]$</td>
<td>$B^{D_{nh}}[l,m]$</td>
<td>None</td>
</tr>
<tr>
<td>$D_{nd}$</td>
<td>$A^{D_{nd}} = A^{D_{nh}}[n]$, $B^{D_{nd}}[l,m,n]$</td>
<td>$B^{D_{nd}}[l,m,n] \rightarrow B^{D_{2nh}}[l,m]$</td>
<td></td>
</tr>
<tr>
<td>$C_{\infty}$</td>
<td>$A^{C_{\infty}}[n]$</td>
<td>None</td>
<td>$A^{C_{\infty}}[n] \rightarrow A^{D_{\infty}}[n]$</td>
</tr>
<tr>
<td>$D_{\infty}$</td>
<td>$A^{D_{\infty}}[n]$</td>
<td>None</td>
<td>None</td>
</tr>
</tbody>
</table>

Note that in these cases we considered situations where the in-plane order has been completely disordered, leading to full $O(2)$ symmetry. Thus the chiral order $\sigma$ for proper groups $C_n$ and $D_n$ has been simultaneously lost. Nevertheless, we can in principle also have the restorations of only the in-plane $SO(2)$ symmetry with the transitions

$$C_n \rightarrow C_{\infty}, \quad D_n \rightarrow D_{\infty}. \tag{5.9}$$

where the chirality $\sigma$ does not disorder [30]. However, since the handedness
field $\sigma$ is a composite of $\{l, m, n\}$ featuring also in-plane ordering, these transitions require more fine tuning in comparison to those in Eq. (5.8).

In the opposite limit, if the in-plane order with order parameter $B$ is sufficiently strong in comparison to the axial ordering $A[n]$, we can disorder the primary axis $n$ without destroying the in-plane order upon increasing the temperature. Note that due to the $O(3)$ constraint, the axial ordering is never fully independent in the presence of the perpendicular in-plane ordering that fixes $n$ up to sign. Therefore, upon disordering the axial order, the symmetry of the phase is augmented by

$$
\sigma_h = \begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & -1
\end{pmatrix},
$$

(5.10)

which is a simply a reflection with respect to the $(l, m)$ plane that acts trivially on the in-plane ordering. Other symmetry operations transforming $n$ to $-n$, such as the inversion or a two-fold rotations about an axis in the $(l, m)$-plane, however, these will simultaneously transform the in-plane order. If such symmetries belong to the original symmetry group $G$, they will lead to enhanced in-plane symmetries in combination with $\sigma_h$. Therefore the new symmetries due to the disordering of the axial order $A^G[n]$ are generated by the elements $\langle G, \sigma_h \rangle$ leading to either the direct product structure $G' \times \{1, \sigma_h\}$ or the semi-direct product $G' \rtimes \{1, \sigma_h\}$, where $G'$ has either $n$-fold or $2n$-fold. These are transitions between phases with different “biaxial” orders $B^G$ and $B^{G^*}$, for convenience to be referred to as biaxial-biaxial* transitions, where superscript in $G^*$ denotes the presence of the additional reflections in comparison with the low temperature symmetries $G$. The behavior of the associated orders in the generalized uniaxial-biaxial transitions Eq. (5.8) and biaxial-biaxial* transition are summarized in Table 5.2.

More specifically for the latter “biaxial-biaxial*” case, since $\sigma_h$ is already contained in the groups $C_{nh}$ and $D_{nh}$, the disordering of the primary axis with order parameter $A^G[n]$ will lead to the phase transition of the
generalized nematics with symmetries \( \{C_n, C_{nv}, S_{2n}, D_n, D_{nh}, D_{nd}\} \)

\[
\begin{align*}
C_n & \rightarrow C_{nh}, \\
S_{2n} & \rightarrow C_{2nh}, \\
C_{nv}, D_n & \rightarrow D_{nh}, \\
D_{nd} & \rightarrow D_{2nh},
\end{align*}
\] (5.11)

as follows from the subgroup structure of \( O(3) \). Since \( \sigma_h \) is already contained in the groups \( C_{nh} \) and \( D_{nh} \), the biaxial* phase is not present for these nematics.

Indeed, we see that these transitions have more interesting features than the generalized uniaxial-biaxial transitions in Eq. (5.8), because \( \sigma_h \) may be “fused” to the parent symmetries via a direct product or semi-direct product, leading to different effects on the original order. For instance, for \( C_n \) and \( C_{nv} \) nematics, whose axial order parameter \( \mathbf{A}^G[n] \) is simply the vector \( \mathbf{n} \), disordering the primary axis in the presence of the in-plane order, i.e. adding the extra symmetry generator \( \sigma_h \), will simply lift this vector to a director. Consequently, the original axial order is destroyed, but a new axial order will persist as long as \( \mathbf{B} \) is ordered and lead to the nematic \( \mathbf{B}^{G^*} \).

Moreover, as given in Eq. (5.4), the axial order parameter for \( D_n \) nematics is already fixed by the in-plane \( C_n \) rotations up to a sign, as well as being invariant under the dihedral \( \pi \)-rotations \( \mathbf{m} \rightarrow -\mathbf{m}, \mathbf{n} \rightarrow -\mathbf{n} \). Therefore, perhaps counter intuitively, upon increasing the temperature and disordering the primary axis, i.e. adding \( \sigma_h \) to the symmetries of the phase, only leads to the vanishing of the chiral order parameter \( \sigma \), while the axial order parameter \( \mathbf{A}[\mathbf{n}] \) is still non-zero, albeit with reduction in its magnitude due to the higher temperature. Last but not the least, in the cases of \( S_{2n} \) and \( D_{nd} \) nematics, since the biaxial order parameter for these symmetries is a function of all the three triads, \( \mathbf{B}^{S_{2n}, D_{nd}} = \mathbf{B}^{S_{2n}, D_{nd}}[l, m, n] \), disordering \( \mathbf{n} \) and promoting \( \sigma_h \) to the axial axis lifts their in-plane structure to a higher in-plane symmetry.

5.2 Gauge theory realization of generalized biaxial transitions

The generalized biaxial transitions in Eq. (5.8) and Eq. (5.11) generalize the biaxial-uniaxial transition of \( D_{2h} \) nematics into a much broader class.
These transitions can be readily realized by a gauge-theoretical description for generalized nematics discussed in Chapter 3. We now recollect the model and show how anisotropic couplings that do not break any symmetries serve as tuning parameters for the generalized nematic phase transitions in Sec. 5.1.2.

**5.2.1 \( O(3)/G \) lattice gauge theory for generalized nematics**

In Chapter 3, we introduced a lattice model to describe nematic orders with an arbitrary three-dimensional point group symmetry. The model is a discrete non-Abelian gauge theory, generalizing from \( Z_2 \) Abelian Lammert-Rokshar-Toner model for \( D_{\infty h} \)-uniaxial nematic liquid crystals [25, 26]. In this model, instead of directly dealing with tensor order parameters, the symmetry of three dimensional nematic orders is realized by a point-group-symmetric gauge theory coupled to \( O(3) \) matrices. Accordingly, the nematic phase and the isotropic phase are realized by the Higgs phase and the confined phase of the gauge theory, respectively. The model is defined by the Hamiltonian [23],

\[
H = H_{\text{Higgs}} + H_{\text{gauge}},
\]

\[
H_{\text{Higgs}} = -\sum_{\langle ij \rangle} \text{Tr} \left[ R_i^T \mathbf{J} U_{ij} R_j \right],
\]

\[
H_{\text{gauge}} = -\sum_{\Box} \sum_{\mathcal{C}_\mu} K_{\mathcal{C}_\mu} \delta_{\mathcal{C}_\mu} (U_{\square}) \text{Tr} \left[ U_{\square} \right].
\]

\( H_{\text{Higgs}} \) is a Higgs term describing interactions between matter fields \( R_i \) and gauge fields \( U_{ij} \). The matter fields \( R_i \)'s live on the sites of a cubic lattice and are defined by the \( O(3) \) matrix in Eq. (5.1). The gauge fields \( U_{ij} \)'s are of the symmetry of \( G \) and live on the link \( \langle ij \rangle \). \( \mathbf{J} \) is a coupling matrix determining how the local axises \( \mathbf{n}_i^a \) interact. This model is invariant under gauge transformations

\[
R_i \rightarrow \Lambda_i R_i, \quad U_{ij} \rightarrow \Lambda_i U_{ij} \Lambda^T_j, \quad \forall \Lambda_i \in G,
\]

which leads to the local identification

\[
R_i \simeq \Lambda_i R_i, \quad \mathbf{n}_i^a \simeq \Lambda_i^{\alpha \beta} \mathbf{n}_i^\beta, \quad \Lambda_i \in G.
\]

Thus \( H_{\text{Higgs}} \) can effectively model the orientational interaction between two \( G \)-symmetric “mesogens”. In addition, \( H_{\text{Higgs}} \) has the global \( O(3) \)-
rotation symmetry

\[ R_i \rightarrow R_i \Omega^T, \quad \Omega \in O(3). \quad (5.17) \]

Since gauge symmetries cannot be broken [28], the fully ordered Higgs phase of \( H_{\text{Higgs}} \) will develop long range order characterized by \( G \)-invariant tensor order parameters and thus realizes spontaneous symmetry breaking of Eq. (5.17) from an isotropic \( O(3) \) liquid phase to a generalized nematic phase with the symmetry \( G \) [23].

\( H_{\text{gauge}} \) describes a point-group-symmetric gauge theory, where

\[ U_{\square} = \prod_{(ij) \in \square} U_{ij} \quad (5.18) \]

denotes the oriented products of gauge fields around plaquettes \( \square \). Plaquettes with non-zero flux \( U_{\square} \neq 1 \) represent gauge defects. Gauge defects in the same conjugacy class are physically equivalent, correspondingly their core energy, \( K_{C_{\mu}} \), is a function of the conjugacy classes \( C_{\mu} \) of the group \( G \). These gauge defects corresponding to the Volterra defects in nematics [23], thus one can in principle turn the topological defects in nematic via assigning these gauge fluxes a finite core energy. However, for the purpose of realizing the generalized biaxial transitions in Eqs. (5.8) and (5.11), the Hamiltonian \( H_{\text{Higgs}} \) is sufficient and for simplicity we will take \( K_{C_{\mu}} = 0 \) in the following.

### 5.2.2 Anisotropic couplings and generalized biaxial transitions

In terms of \( n_i^\alpha = \{l_i, m_i, n_i\} \), we can define a local triad vector \( n_j^{\beta\gamma} = U_{ij}^{\beta\gamma} n_j^\gamma \) at a site \( j \), which has been brought ("parallel transported") into the same local gauge as \( n_i^\alpha \) at the site \( i \), and express \( H_{\text{Higgs}} \) as

\[
H_{\text{Higgs}} = - \sum_{(ij)} n_i^\alpha \cdot J_{ij}^{\alpha\beta} (U_{ij})^{\beta\gamma} n_j^\gamma \\
= - \sum_{(ij)} J_{ij}^{\alpha\beta} n_i^\alpha \cdot n_j^{\beta\gamma}.
\quad (5.19)
\]

This shows explicitly that \( J_{ij}^{\alpha\beta} \) parametrizes the interaction between two local triads.
Table 5.3. Classification the coupling matrix $\mathbf{J}$. The coupling matrix $\mathbf{J}$ needs to be invariant under a given three-dimensional point group $G$, $\Lambda \mathbf{J} \Lambda^T = \mathbf{J}$, $\forall \Lambda \in G$. The possible forms of $\mathbf{J}$ can be found in from a standard textbook for solid state physics, e.g., Ref. [137].

<table>
<thead>
<tr>
<th>Symmetry Groups</th>
<th>Coupling Matrix</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_1, C_i \cong S_2$</td>
<td>$\begin{pmatrix} J_1 &amp; J_{12} &amp; J_{13} \ J_{12} &amp; J_2 &amp; J_{23} \ J_{13} &amp; J_{23} &amp; J_3 \end{pmatrix}$</td>
</tr>
<tr>
<td>$C_s \cong C_{1h} \cong C_{1v}$, $C_2, C_{2h}$</td>
<td>$\begin{pmatrix} J_1 &amp; J_{13} \ J_2 \ J_{13} &amp; J_3 \end{pmatrix}$</td>
</tr>
<tr>
<td>$C_{2v}, D_2, D_{2h}$</td>
<td>$\begin{pmatrix} J_1 \ J_2 \ J_3 \end{pmatrix}$</td>
</tr>
<tr>
<td>$C_{n \geq 3}, C_{(n \geq 3)v}$, $S_{2(n \geq 2)}, C_{(n \geq 3)h}$, $D_{n \geq 3}$, $D_{(n \geq 3)h}$, $D_{(n \geq 2)d}$</td>
<td>$\begin{pmatrix} J_1 \ J_1 \ J_3 \end{pmatrix}$</td>
</tr>
<tr>
<td>$T, T_d, T_h$, $O, O_h, I, I_h$</td>
<td>$\begin{pmatrix} J \ J \ J \end{pmatrix}$</td>
</tr>
</tbody>
</table>
Moreover, \( \mathbf{J} \) has to respect the symmetry of the underlying “mesogens” (order parameter fields). In the language of the gauge theory, it needs to satisfy the constraint

\[
\Lambda \mathbf{J} \Lambda^T = \mathbf{J}, \quad \forall \Lambda \in G
\]

for a given gauge group \( G \). This heavily restricts the possible forms of \( \mathbf{J} \). These possible forms can be found from a standard textbook for solid state physics like Ref. [137], and we tabulate the results in Table 5.3 for the convenience of the reader.

Table 5.3 shows that anisotropic couplings are allowed for axial nematics. This anisotropy is hardwired in the gauge theory Eq. (5.12) and do not break any additional symmetries. Although we have fixed the local point group action, i.e. the gauge symmetries, in terms of the triads \{\mathbf{l}, \mathbf{m}, \mathbf{n}\}, we can always diagonalize the symmetric matrix \( \mathbf{J}^{\alpha \beta} \) by a global redefinition \( R_i \to DR_i, \quad U_{ij} \to DU_{ij}D^T \). Inspecting the allowed matrices \( \mathbf{J} \), the only non-trivial case are the simple monoclinic symmetries \( (C_\infty, C_2, C_{2h}) \), since in the case of \( C_1 \) and \( C_i \simeq S_2 = \{1, -1\} \), there are no rotational gauge symmetries \( U_{ij} \) to begin with. It is easy to see that the monoclinic symmetries only introduce a common \( \pm \) sign in the \( (\mathbf{l}, \mathbf{m}) \)-plane with the non-diagonal couplings. Therefore without loss of generality we can diagonalize the couplings,

\[
\mathbf{J} = \begin{pmatrix}
J_1 \\
J_2 \\
J_3
\end{pmatrix}
\]

with \( J_1, J_2, J_3 \geq 0 \) for nematic alignment. For the monoclinic symmetries, this requires \( J_{13} \leq \sqrt{J_1 J_3} \) and we do not consider negative or “antineumatic” couplings [138, 139].

The line of thought can actually be reversed in the sense that we can take couplings \( J_1, J_2, J_3 \) be a measure of the three dimensionality of the “mesogens”. One realizes that they provide tuning parameters for the phase transitions involving the axial and in-plane ordering. For the purpose of realizing the transitions in Eq. (5.8) and Eq. (5.11), we can
consider the following form for simplicity,

\[
\beta \mathbf{J} = \beta \begin{pmatrix} J_1 \\ J_1 \\ J_3 \end{pmatrix} = \beta J_3 \begin{pmatrix} J_1 \\ J_3 \\ 1 \end{pmatrix} = \beta J_1 \begin{pmatrix} 1 \\ 1 \\ J_3/J_1 \end{pmatrix},
\]

where \( J_1 \) specifies the coupling of the in-plane degrees of freedom and \( J_3 \) the coupling between the primary axes. Therefore this form of \( \mathbf{J} \) is allowed for all axial groups and quantifies the anisotropy between the in-plane order and axial order, as the situation considered in Section 5.1.1.

The fact that the phase transitions are tuned with respect to the inversed temperature \( \beta = 1/T \) reduces the the independent dimensionless couplings to two in terms of \( \beta \) and the anisotropy \( J_1/ J_3 \) or \( J_3/ J_1 \). The ratio \( J_1/ J_3 \), or equivalently \( J_3/ J_1 \), is in fact an analogue to the so-called biaxiality parameter of \( D_{2h} \) nematics [140–142, 71]. Accordingly, when \( J_1/ J_3 \) is sufficiently small, upon increasing temperature we expect that the in-plane order will be lost while the axial order still persist, leading to the generalized biaxial-uniaxial transition given in Eq. (5.8). In the opposite limit, where \( J_3/ J_1 \) is sufficiently large, it is possible to disorder the axial order while the in-plane order is still maintained, leading to the generalized biaxial-biaxial* transitions characterized by Eq. (5.11). Between these two limiting cases we expect direct transitions from the biaxial nematics to the \( O(3) \) isotropic liquid. Note however that in general the “biaxial” in-plane order is much more fragile than the uniaxial order of the primary axial axis. Furthermore, the biaxial in-plane order reinforces the uniaxial order since it fixes the perpendicular axial order up to a sign. Conversely, the presence of the axial order reinforces the biaxial order much less, since ordering along \( \mathbf{n} \) still leaves in-plane \( SO(2) \) fluctuations before the full ordering sets in. As has been discovered in Chapter 3, the highly symmetric order parameter fields experience giant fluctuations and generalized biaxial nematics with a more symmetric in-plane structure require much
larger $\frac{J_1}{J_3}$ to stabilize the in-plane order.

Nevertheless, although $\frac{J_1}{J_3}$ parameterizes the anisotropy of the in-plane and axial order of general biaxial nematics, they are defined in the gauge theory, so their values do not directly describe the relative strength of the in-plane order and axial order. Therefore $\frac{J_1}{J_3} > 1$ does not necessary mean the in-plane order is favored, and vice versa. Moreover, in the gauge theoretical effective Hamiltonian Eq. (4.7) terms respecting all the symmetries appear order by order. Due to the $O(3)$ relations Eqs. (5.1) and (5.2), naturally only two of the orthonormal triads are fully independent. Therefore gauge invariant interactions such as $(l_i \times m_i) \cdot (l_j \times m_j) = \sigma_i \sigma_j n_i \cdot n_j$ or $(l_i \cdot l_j)^2 + (m_i \cdot m_j)^2 + (m_i \cdot l_j)^2 \approx (n_i \cdot n_j)^2$ will be present with coefficients parametrized by powers of $J_1$. Consequently, even though $J_3 = 0$, effective axial interactions $J_{3,\text{eff}}(J_1) \sigma_i \sigma_j n_i \cdot n_j$ or $J'_{3,\text{eff}}(J_1) (n_i \cdot n_j)^2$ will be generated if allowed by the symmetries. In particular this affects higher order axial symmetries that have high rank order parameter tensors with large fluctuations.

5.2.3 Temperature-anisotropy phase diagrams

Based on the discussions in Sections 5.1.2 and 5.2.2, we can now sketch the phase diagrams of biaxial nematics at different temperatures and anisotropies of $\mathbf{J}$ defined in Eq. (5.22). For simplicity, here we will restrict us to axial nematics whose in-plane structure is not very symmetric, so the induced effective axial coupling is not quite relevant. However, in the Appendix 5.A we will briefly discuss situations of highly symmetric axial nematics and the effect of the induced axial coupling.

The phase diagrams with respect to $\frac{J_1}{J_3}$ and $\frac{J_3}{J_1}$ are shown in Fig. 5.1 and Fig. 5.2, respectively. Since $\frac{J_1}{J_3}$ and $\frac{J_3}{J_1}$ are equivalent in measuring the anisotropy of $\mathbf{J}$, these two phase diagrams should be consistent.

Firstly, they should give the same phases and phase transitions. Concretely, in the $\frac{J_3}{J_1}$ phase diagram Fig. 5.1, we expect the generalized biaxial-uniaxial transitions in Eq. (5.8) to happen at small $\frac{J_1}{J_3}$, and the generalized biaxial-biaxial transitions of Eq. (5.11) happen at large $\frac{J_1}{J_3}$. These phase transitions should respectively appear at large $\frac{J_3}{J_1}$ and small $\frac{J_1}{J_3}$ in the $\frac{J_1}{J_3}$ phase diagram Fig. 5.2.

Secondly, the anisotropies of $\mathbf{J}$ should also be consistent in these two types of phase diagrams. In the $\frac{J_3}{J_1}$ and $\frac{J_1}{J_3}$ phase diagrams, we can define a critical anisotropy $(\frac{J_1}{J_3})^U$ and $(\frac{J_3}{J_1})^U$ where the biaxial-uniaxial transition
Figure 5.1. The schematic temperature-anisotropy phase diagrams for the axial nematics with not very large $n$, as a function of $\frac{J_1}{J_3}$. Small and large $\frac{J_1}{J_3}$ correspond to weak and strong in-plane coupling, respectively. $(\frac{J_1}{J_3})_c^U$ and $(\frac{J_1}{J_3})_c^B$ are the critical anisotropy where the generalized biaxial-uniaxial transitions in Eq. (5.8) and the biaxial-biaxial* transitions in Eq. (5.11) terminate, respectively. Solid lines in the figure are for all axial symmetries $\{C_n, C_{nv}, S_{2n}, C_{nh}, D_n, D_{nh}, D_{nd}\}$, while the dashed line is only for symmetries $\{C_n, C_{nv}, S_{2n}, D_n, D_{nd}\}$.

Figure 5.2. The schematic temperature-anisotropy phase diagrams for the axial nematics with not very large, as a function of $\frac{J_3}{J_1}$. Similarly to Fig. 5.1, but small and large $\frac{J_3}{J_1}$ correspond to strong and weak in-plane coupling, respectively.
line terminates, respectively. These two critical anisotropies should satisfy
\[
(J_3/J_1)^U_c = [(J_3/J_1)^U_c]^{-1},
\]
(5.23)
since they correspond to the same anisotropy of $\mathbf{J}$. A critical anisotropy for the generalized biaxial-biaxial* transition can be defined in a similar way, as $(J_1/J_3)^B_c$ and $(J_3/J_1)^B_c$, and they in turn satisfy
\[
(J_3/J_1)^B_c = [(J_3/J_1)^B_c]^{-1}.
\]
(5.24)

Moreover, as we discussed in Section 5.2.2, biaxial nematics with a more symmetric in-plane structure require larger $J_1$ to stabilize the in-plane order. The critical anisotropy $(J_3/J_1)^U_c$ for the uniaxial-biaxial transitions in the $J_3$ phase diagram Fig. 5.1 will therefore move to the right for biaxial nematics with a larger in-plane $n$-fold rotational symmetry or having more reflection planes acting on in-plane axes. One the other hand, since a weaker in-plane order in turn means a stronger axial order, the critical anisotropy $(J_1/J_3)^B_c$ for the biaxial-biaxial* transitions will correspondingly move to the right. Accordingly, in these critical anisotropies of $\mathbf{J}$ will move to the opposite direction in the $J_3$ phase diagram Fig. 5.2.

Lastly, although the gauge theoretical formulation is not realized microscopically in any condensed matter system, it encodes the mesogenic symmetries very efficiently and we expect the qualitative features and the topology of the phase diagrams to be applicable to many generalized nematic systems. This is clear from the biaxial-uniaxial phase diagrams for symmetries $D_2$ and $D_{2h}$, where all expected features of the mean-field phase diagram are recovered [140, 71], as will be discussed in more detail in Section 5.3.

### 5.3 Monte-Carlo simulations

We have simulated the $J_3/J_1$ and $J_1/J_3$ phase diagrams shown in Figs. 5.1 and 5.2 for nematics with symmetries $\{S_2, C_2, C_{2v}, C_{2h}, D_2, D_{2h}, D_{2d}\}$ which covers all types of axial symmetries. Moreover, we also checked the phase transitions in Eqs. (5.8) and (5.11) for many higher symmetries such as $S_4$, $C_{3v}$, $D_3$, $D_{3h}$, $D_4$, $D_{4h}$, $D_6$ and $D_{6h}$. We used the standard Metropolis Monte-Carlo algorithm, and the simulations were performed on lattices with the size $L^3 = 10^3, 12^3, 16^3$. Our results agree with the above scenario of generalized biaxial phase transitions.
Table 5.4. Generalized biaxial phase transitions for \( \{S_2, C_2, C_{2v}, C_{2h}, D_2, D_{2h}, D_{2d}\} \) nematics. The first column specifies the symmetries and the second column specifies the type of the phase transition. The third and fourth column give the orders which have been destroyed and survive during the phase transition. The explicit form of the associated order parameters can be found in Table 5.1.

<table>
<thead>
<tr>
<th>Symmetry Groups</th>
<th>Phase Transitions</th>
<th>Order Destroyed</th>
<th>Order Remained</th>
</tr>
</thead>
<tbody>
<tr>
<td>( S_2 )</td>
<td>( S_2 \rightarrow C_{2h} )</td>
<td>( B_2^{S_2}, B_3^{S_2} )</td>
<td>( A^{D_{\infty h}}, B_1^{S_2} = B^{C_{2h}} )</td>
</tr>
<tr>
<td></td>
<td>( S_2 \rightarrow D_{\infty h} )</td>
<td>( B^{S_2} )</td>
<td>( A^{D_{\infty h}} )</td>
</tr>
<tr>
<td></td>
<td>( S_2 \rightarrow O(3) )</td>
<td>( A^{D_{\infty h}}, B^{S_2} )</td>
<td>None</td>
</tr>
<tr>
<td>( C_2 )</td>
<td>( C_2 \rightarrow C_{2h} )</td>
<td>( \sigma )</td>
<td>( A^{C_{\infty v}}, B^{C_2} = B^{C_{2h}} )</td>
</tr>
<tr>
<td></td>
<td>( C_2 \rightarrow C_{\infty v} )</td>
<td>( B^{C_2}, \sigma )</td>
<td>( A^{C_{\infty v}} )</td>
</tr>
<tr>
<td></td>
<td>( C_2 \rightarrow O(3) )</td>
<td>( A^{C_{\infty v}}, B^{C_2}, \sigma )</td>
<td>None</td>
</tr>
<tr>
<td>( C_{2v} )</td>
<td>( C_{2v} \rightarrow D_{2h} )</td>
<td>( A^{C_{\infty v}} )</td>
<td>( A^{D_{\infty h}}, B^{C_{2v}} = B^{D_{2h}} )</td>
</tr>
<tr>
<td></td>
<td>( C_{2v} \rightarrow C_{\infty v} )</td>
<td>( B^{C_{2v}} )</td>
<td>( A^{C_{\infty v}} )</td>
</tr>
<tr>
<td></td>
<td>( C_{2v} \rightarrow O(3) )</td>
<td>( A^{C_{\infty v}}, B^{C_{2v}} )</td>
<td>None</td>
</tr>
<tr>
<td>( C_{2h} )</td>
<td>( C_{2h} \rightarrow D_{\infty h} )</td>
<td>( B^{C_{2h}} )</td>
<td>( A^{D_{\infty h}} )</td>
</tr>
<tr>
<td></td>
<td>( C_{2h} \rightarrow O(3) )</td>
<td>( A^{D_{\infty h}}, B^{C_{2h}} )</td>
<td>None</td>
</tr>
<tr>
<td>( D_2 )</td>
<td>( D_2 \rightarrow D_{2h} )</td>
<td>( \sigma )</td>
<td>( A^{D_{\infty h}}, B^{D_2} = B^{D_{2h}} )</td>
</tr>
<tr>
<td></td>
<td>( D_2 \rightarrow D_{\infty h} )</td>
<td>( B^{D_2}, \sigma )</td>
<td>( A^{D_{\infty h}} )</td>
</tr>
<tr>
<td></td>
<td>( D_2 \rightarrow O(3) )</td>
<td>( A^{D_{\infty h}}, B^{D_2}, \sigma )</td>
<td>None</td>
</tr>
<tr>
<td>( D_{2h} )</td>
<td>( D_{2h} \rightarrow D_{\infty h} )</td>
<td>( B^{D_{2h}} )</td>
<td>( A^{D_{\infty h}} )</td>
</tr>
<tr>
<td></td>
<td>( D_{2h} \rightarrow O(3) )</td>
<td>( A^{D_{\infty h}}, B^{D_{2h}} )</td>
<td>None</td>
</tr>
<tr>
<td>( D_{2d} )</td>
<td>( D_{2d} \rightarrow D_{4h} )</td>
<td>( B^{D_{2d}} )</td>
<td>( A^{D_{\infty h}}, B^{D_{4h}} )</td>
</tr>
<tr>
<td></td>
<td>( D_{2d} \rightarrow D_{\infty h} )</td>
<td>( B^{D_{2d}} )</td>
<td>( A^{D_{\infty h}} )</td>
</tr>
<tr>
<td></td>
<td>( D_{2d} \rightarrow O(3) )</td>
<td>( A^{D_{\infty h}}, B^{D_{2d}} )</td>
<td>None</td>
</tr>
</tbody>
</table>
5.3.1 Determination of the phases

To determine the symmetry of a nematic phase with the tensor order parameter \( O^G \), one in principle needs to consider all the entries of \( O^G \). However, for interactions favoring homogeneous distribution of the order parameter fields, such as the interaction in the gauge model Eq. (5.12), the symmetry of the phase can be revealed by the strength of the ordering which is a scalar order parameter defined as

\[
q = \sqrt{\langle O_{abc...}^G \rangle^2}, \tag{5.25}
\]

where \( O^G = \frac{1}{L^3} \sum_i O_i^G \) averages over the system and contractions for repeated indexes are assumed. This nematic ordering strength will develop a finite value in the ordered phase and vanish in the disordered phase (For more details of this method see Chapter 4.).

For axial nematics, we accordingly need to define the ordering strength for the axial order \( A^G \) and the in-plane order \( B^G \), respectively,

\[
q_A = \sqrt{\langle A_{ab..}^G \rangle^2}, \tag{5.26}
\]
\[
q_B = \sqrt{\langle B_{ab..}^G \rangle^2}. \tag{5.27}
\]

A transition is then identified by the peak of the associated susceptibility

\[
\chi(q_{A,B}) = \frac{L^3}{T} \left( \langle q_{A,B}^2 \rangle - \langle q_{A,B} \rangle^2 \right). \tag{5.28}
\]

where \( \langle \ldots \rangle \) denotes the thermal average.

In addition, we also computed the heat capacity and the susceptibility of the chiral order parameter, which are defined as the usual way,

\[
C_v = \frac{1}{T^2 L^3} (\langle E^2 \rangle - \langle E \rangle^2), \tag{5.29}
\]
\[
\chi(\sigma) = \frac{L^3}{T} (\langle \sigma^2 \rangle - \langle \sigma \rangle^2). \tag{5.30}
\]

where \( E \) is the internal energy of the system, and \( \sigma = \frac{1}{L^3} \sum_i \sigma_i \) is the global chiral order parameter.

5.3.2 Numerical phase diagrams

Although \( J_1 \) and \( J_3 \) are equivalent in describing the anisotropy of the coupling matrix \( J \) in Eq. (5.22), there is nevertheless a preference for
one or the other in practical simulations. We aimed at the generalized biaxial-uniaxial transitions in Eq. (5.8) by the \( J_1/J_3 \) phase diagram, since the biaxial* phase may require extremely large \( J_1/J_3 \) and is in general difficult to access in the \( J_1/J_3 \) phase diagram. On the other hand, we used the \( J_1/J_3 \) phase diagram to discuss the generalized biaxial-biaxial* transitions.

The results are presented in Figs. 5.3 – 5.8. The associated order parameters and their behaviors in the phase transitions are collected in Table 5.1 and Table 5.4, respectively.

These phase diagrams correctly give the expected phase and phase transitions, including the well known biaxial-uniaxial transition of \( D_{2h} \) and \( D_2 \) nematics [140–142]. Particularly, in the \( J_1/J_3 \) phase diagram for \( D_2 \) nematics in Fig. 5.4(a), we find that the transition between the \( D_2 \)-biaxial nematic phase and the \( O(3) \) isotropic liquid phase is first-order like. Both \( \chi(q_B) \), \( \chi(\sigma) \) and \( C_v \) exhibit a sudden peak at this transition, and the magnitude of their peak grows dramatically with the lattice size. This discontinuity continues to the biaxial-uniaxial transition line. Therefore, at where the three transition lines in Fig. 5.4(a) meet, we identify a triple point that the three phases can coexist. Moreover, in the middle of the biaxial-uniaxial transition line we find evidence for a tricritical point where the first order phase transition terminates and the transition becomes continuous. These observation agree with the experiments results of
**Figure 5.4.** Temperature-anisotropy phase diagrams of $D_2$ nematics as a function of $\frac{J_1}{J_3}$ (a) and $\frac{J_3}{J_1}$ (b). In addition to a biaxial-liquid transition, there is a $D_2 \rightarrow D_{2h}$ biaxial-biaxial$^*$ transition at the large $\frac{J_1}{J_3}$ region.

**Figure 5.5.** Temperature-anisotropy phase diagrams of $S_2$ nematics as a function of $\frac{J_1}{J_3}$ (a) and $\frac{J_3}{J_1}$ (b). The $S_2 \rightarrow D_{\infty h}$ biaxial-uniaxial transition at small $\frac{J_1}{J_3}$ region and the $S_2 \rightarrow C_{2h}$ biaxial-biaxial$^*$ transition at large $\frac{J_1}{J_3}$ region are shown by (a) and (b), respectively.
Figure 5.6. Temperature-anisotropy phase diagrams of $C_2$ nematics as a function of $J_1/J_3$ (a) and $J_3/J_1$ (b). The $C_2 \rightarrow C_{2h}$ biaxial-biaxial* transition is only shown in the $J_3/J_1$ phase diagram for practical convenience.

Moreover, these numerical phase diagrams demonstrate the consistency of the critical anisotropic couplings discussed in Section 5.2.3. Take the $D_2$ nematic as an example. As can be seen from Fig. 5.4(a), the critical anisotropy for the uniaxial-biaxial transition in the $J_3/J_1$ phase diagram in Fig. 5.4(a) is $(J_3/J_1)^U_c \sim 0.6$. Consistently, the same anisotropy in the $J_3/J_1$ phase diagram in Fig. 5.4(b) is given by $(J_3/J_1)^U_c \sim 1.7$, satisfying Eq. (5.23).

Although we only show results for a small set of axial nematics, we can already see the tendency of the value of the critical anisotropies with respect to the in-plane symmetry of the order. Take $D_2$ and $D_{2d}$ nematics as an example. These orders have the same axial structure, while the $D_{2d}$ order has a four-fold in-plane rotational symmetry, as compared to the two-fold rotational symmetry in the $D_2$ phase. Therefore, we expect the critical anisotropies $(J_3/J_1)^U_c$ and $(J_3/J_1)^B_c$ of the $D_2$ order to be larger than those in the $D_{2d}$ case, which is indeed the case in Fig. 5.4(b) and Fig. 5.8(b). As another example, both $C_2$ and $D_2$ symmetry have a two-fold in-plane rotations. However, the latter one is more symmetric in its axial order. This in turn means that the axial order in the $C_2$ case is stronger relative to its in-plane order. Therefore, we expect the critical anisotropies $(J_3/J_1)^U_c$ and $(J_3/J_1)^B_c$ of the $C_2$ order to be smaller than those in the $D_2$ order, as compared to those in the $D_2$ case, which is indeed the case in Figs. 5.6(b) and 5.4(b).
Figure 5.7. Temperature-anisotropy phase diagrams of $C_{2v}$ nematics as a function of $J_3/J_1$ (a) and $J_1/J_3$ (b). The $C_{2v} \rightarrow D_{2h}$ biaxial-biaxial* transition is only shown in the $J_3/J_1$ phase diagram for practical convenience.

Figure 5.8. Temperature-anisotropy phase diagrams of $D_{2d}$ nematics as a function of $J_3/J_1$ (a) and $J_1/J_3$ (b). The $D_{2d} \rightarrow D_{4h}$ biaxial-biaxial* transition is only shown in the $J_3/J_1$ phase diagram for practical convenience.
5.4 Concluding remarks

There is a rich landscape of unexplored generalized nematics, entailing not only a diversity of orientational phases in terms of their symmetry but also an abundance in possible vestigial phases. In this chapter, we have discussed the anisotropy-induced vestigial uniaxial and biaxial phases for nematics characterized by axial point-group symmetries and studied their phase transitions. Our results generalize the well-studied biaxial-uniaxial transition of $D_{2h}$ nematics to a much broader class, that can be directly accessed within our earlier proposed gauge theoretical formulation of generalized nematics and follow from a-priori symmetry arguments. This framework allows us in particular to compare nematics and vestigial phases with different symmetries in one common reference. Utilizing this formalism, we found that, in comparison to the familiar $D_{2h}$ biaxial nematic phase, nematic phases with high axial symmetries require much lower temperature to stabilize their order. This motivates the fact that biaxial phases with high symmetry are difficult to realize in reality and have not yet been experimentally encountered: before reaching the low temperature demanded by the biaxial order, crystallization may already start playing a role. Consequently, columnar, smectic and/or crystalline phases may occur instead of a generalized nematic phase. These challenges notwithstanding, the advances in the fabrication and manipulation of colloidal systems of nanoparticles appear in fact promising with regards to stabilizing generalized nematic phases in the laboratory in the near future [80, 77, 81, 78, 83].

Besides these generalized biaxial transitions, there may be more vestigial phases and transitions in the gauge model Eq. (5.12). Those phases are associated with the defects in the model, which have been ignored in this work by setting $H_{\text{gauge}} = 0$ in Eq. (5.12), describing the confined and Higgs phases of the model. From the point of view of topological melting, phase transitions may be understood as a proliferation of topological defects [26, 30, 31]. To illustrate this further we can take the $D_{2h}$-biaxial nematic as an example. According to homotopy theory, topological defects of $D_{2h}$ nematics are classified by the five conjugacy classes of the quaternion group $Q_8$ [143, 19, 20, 116]. Among these defects, there are only three elementary ones, which are the $\pi$-disclinations in the three orthogonal planes of the three dimensional space. In the transition of the nematic phase to the $O(3)$ liquid phase, all these defects proliferate. In the biaxial-uniaxial transition, however, one of them stays gapped. This
implies that a phase transition can be affected by the tuning of the energy cost of topological defects. The gauge model Eq. (5.12) provides a natural way to do this. Concretely, when the $H_{\text{gauge}}$ term is set to be zero, topological defects in the model only cost elastic energy by the $H_{\text{Higgs}}$ term. By tuning on the $H_{\text{gauge}}$ term, however, we can introduce a finite core energy to a particular class of topological defects, and therefore modify the nature of the phase transition. While such defect terms $H_{\text{gauge}} \neq 0$ have been identified to be important in the melting of many quantum nematics [60, 61, 58, 59, 16, 144], they have not yet been discovered to play a role in the realm of classical nematics and melting [145]. The rich physics associated with these ideas leave many interesting avenues of for future research in the generalized nematic systems.
5.A Phase diagrams for axial nematics with high symmetries

So far we have focused on axial nematics with a not very symmetric in-plane structure, where the induced axial coupling does not have profound effects. For axial nematics with high symmetries, the induced axial coupling becomes more relevant and may stabilize a uniaxial phase always before the underlying biaxial phase. Here we will briefly discuss the general feature of these situations. For more details, see Ref. [32].

In Fig. 5.9, we show the $J_1-J_3$ phase diagram for $D_{2h}$, $D_{3h}$ and $D_{4h}$ nematics. Let us first focus on the $D_{2h}$ case in Fig. 5.9(a). As in the temperature-anisotropy phase diagram in Fig. 5.3(a), in the region with small $J_1$ and large $J_3$ there is a vestigial uniaxial phase sandwiched between the fully ordered biaxial phase and the disordered liquid phase. The critical anisotropy where the vestigial uniaxial phase starts appearing is consistent with that of Fig. 5.3(a), up to our numerical accuracy. Moving to $D_{3h}$ case, the increased in-plane symmetry requires a larger in-plane coupling (lower temperature and larger $J_1$ anisotropy) to stabilize the biaxial order, due to the more severe fluctuations. The biaxial phase is therefore squeezed by the liquid phase and the vestigial uniaxial phase.

The squeezing of the biaxial phase is even more prominent for the $D_{4h}$ nematics, where the in-plane symmetry is increased further. In particular, since very large in-plane coupling is required to stabilize the highly symmetric $D_{4h}$ order, before the biaxial phase is realized, the induced axial coupling is always sufficiently strong for the uniaxial order. This leads to a vestigial uniaxial phase realized for all non-negative values of the “bare” axial coupling $J_3$, while the direct biaxial-liquid transition is absent. The same is true for the more symmetric $D_{6h}$ nematics, with a even larger region of the vestigial uniaxial phase.

However, one should not interpret this as a no-go theorem for a direct biaxial-liquid transition in the case of highly symmetric biaxial nematics. Instead, this simply means that in order to realize this transition, one needs to consider a model with “anti-nematic” coupling for the axial order to offset the induced axial coupling.

The above discussions can similarly be verified for $D_2$, $D_3$ and $D_4$ nematics as well, as shown in Fig. 5.10. Nonetheless, since the biaxial-biaxial* transition is possible for these cases, in the small $J_3$ region, there is in addition a vestigial biaxial* phase. This phase is also squeezed as
Figure 5.9. The $J_1$-$J_3$ phase diagram of (a) $D_{2h}$, (b) $D_{3h}$ and (c) $D_{4h}$ nematics. Similar to the temperature-anisotropy phase diagram in Fig. 5.3(a), there is a vestigial uniaxial phase appearing from the region with small $J_1$ and large $J_3$ (small $\frac{J_1}{J_3}$), realizing the generalized biaxial-uniaxial transition in Eq. (5.8). As the symmetry increases, this vestigial uniaxial phase becomes more prominent and the fully ordered biaxial phase is remarkably squeezed. When the symmetry is sufficiently high, the vestigial uniaxial phase appears adjacent to the isotropic liquid due to the symmetry allowed axial terms. The red star in the $D_{2h}$ and $D_{3h}$ case highlights a tricritical/triple point where the three transition lines meet.
Figure 5.10. The $J_1$-$J_3$ phase diagram of $D_2$ (a), $D_3$ (b) and $D_4$ (c) nematics. Similar to Fig. 5.9, but there is in addition a vestigial biaxial* phase at small $J_3$ region, realizing the generalized biaxial-biaxial* transition in Eq. (5.11). Both this vestigial biaxial* phase and the fully ordered biaxial phase are squeezed considerably as the symmetry increases. The associated tricritical/triple points at where transition lines meet are highlighted by large stars.
symmetries increase, as in the case of the fully ordered biaxial phase. Moreover, in cases of $D_2$ and $D_3$, there are direct transitions from the fully ordered biaxial phase or vestigial biaxial phase to the liquid phase. For the highly symmetric $D_4$ case, however, these transitions are replaced by a biaxial-uniaxial or a biaxial*-uniaxial transition, since a vestigial uniaxial phase exists for all non-negative values of $J_3$ as in the $D_{4h}$ case due to the induced axial couplings.