Gauge theory and nematic order : the rich landscape of orientational phase transition

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Chapter 4

Classification of $3D$ point-group-symmetric order parameter tensors

Rotational symmetry breaking of the three dimensional (3D) orthogonal group $O(3)$ plays an important role in many condensed matters systems, from classical and quantum spins to molecular and strongly correlated electronic nematic liquids [17, 11, 118, 119]. In familiar instances, like the Heisenberg ferromagnet and the uniaxial nematic, the full rotational group $O(3)$ is broken to $O(2)$ and $D_{\infty h}$, respectively. However these are in fact only two special cases of the rich landscape of $O(3)$ symmetry breaking. Indeed, as a matter of principle, matter can break the rotational symmetries of isotropic space $O(3)$ to any of its subgroups, leading to long range orientational order characterized by complicated tensors order parameters.

The subgroups of $O(3)$ have been mathematically identified for a long time, however, it appears that the zoo of point-group orientational orders has never been explored in full generality. Needless to say, the classification of rotational order parameters for some non-broken symmetries has been gradually accumulating since the past century due to various motives. Firstly, in the soft matter literature the unixial ($D_{\infty h}$) and biaxial (D_{2h}) order parameter have been shown to be characterized by second-rank tensors [11], which have been intensively studied in various theories [72–74, 71, 86, 75, 120, 93]. In addition, higher rank ordering tensors for the T_d-tetrahedral [89–91, 97], O_h-cubic [18, 88, 96] and I_h-icosahedral [121–123, 88, 89, 124] orders have been discussed by many authors e.g. in the context of Landau theories and nematic lattice models. Nonetheless, these cover still only a small subset of all 3D point group symmetries and, to the best of our knowledge, the order parameters for most instances are not known explicitly nor have they appeared within a single unified classification scheme. These general order parameters, however, are becoming of more practical interest. New exotic orientational orders may be realized in ensembles of anisotropic constituents, especially nano- and colloidal particles of different shapes [81, 82]. In particular, the increasing experimental ability to control such degrees of freedom [80, 125, 126, 78] is especially promising in this regard. Secondly, many unconventional orientational orders have also been proposed for quantum magnets [127, 128, 116] and spinor condensates [129, 130]. In all these cases, the order parameters associated with each symmetry are indispensable to eventually verify the symmetry of these phases and the associated physics.

Now we will use the gauge theory we introduced in Chapter 3.1 to develop a systematic way of deriving the tensor order parameter with arbitrary point groups. In particular, we will highlight the order parameters for physically interesting symmetries including all the crystallographic point groups, the icosahedral groups arising in the context of quasi-crystalline ordering, and the five infinite axial groups $\{C_\infty \simeq SO(2), C_{\infty v} \simeq O(2), C_{\infty h}, D_\infty, D_{\infty h}\}$ exhibiting a continuous rotational $SO(2)$-axis. We show that in order to uniquely characterize a point-group-symmetric orientational order of a phase, at most two order parameter tensors and a pseudoscalar are needed: the second ordering tensor is required by the finite axial groups $\{C_n, C_{nv}, S_{2n}, C_{nh}, D_n, D_{nh}, D_{nd}\}$, whereas the pseudoscalar chiral order parameter is a requisite associated with the handedness or chirality of the proper point groups $\{C_n, D_n, T, O, I\}$ that are subgroups of the group of proper three-dimensional rotations $SO(3)$.

4.1 Construction of orientational ordering tensor

4.1.1 Warm up: Heisenberg ferromagnetic order and uniaxial nematic order

Let us begin by recalling the characterization of rotational ordering in the familiar context of the Heisenberg ferromagnet and the conventional uniaxial nematic.

In the ferromagnetic phase of a classical Heisenberg magnet, the rotational $O(3)$ symmetry of the Hamiltonian breaks down to the point group $C_{\infty v} \simeq O(2)$ defined by the axis of magnetization $\mathbf{M}$. The order parameter $\mathbf{M} = \langle \mathbf{n}_i \rangle$ is given by the macroscopic averaging of local spins $\mathbf{n}_i$ and is a 3D vector with an orientational order parameter space $O(3)/O(2) \simeq S^2$.

On the other hand, for uniaxial liquid crystals or spin nematics, where

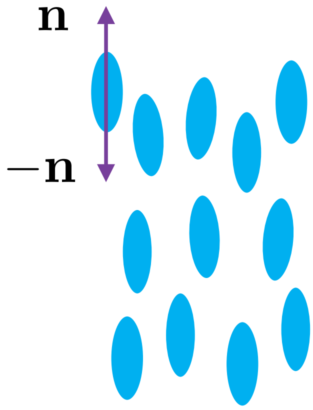

Figure 4.1. Sketch of $D_{\infty h}$ uniaxial molecules. The orientation of a molecule can be defined by a single axis.

the $O(3)$ symmetry is broken to the point group $D_{\infty h}$ in the ordered phase, the system exhibits a macroscopic ordering along an axis $\mathbf{n}$. The uniaxial symmetry $D_{\infty h}$ acts on the order parameter as $\mathbf{n} \to -\mathbf{n}$ and these describe the same macroscopic ordering. Often depicted as being formed of explicitly rod-like "molecules" (Fig. 4.1), a coarse-grained order parameter can be formulated in terms of a local vector $\mathbf{n}_i$ along the "long" axis of each "molecule", with the identification of $\mathbf{n}_i$ with $-\mathbf{n}_i$. To define the uniaxial orientational order, one therefore needs a second rank tensor, $\mathbb{Q}[\mathbf{n}] = \mathbf{n} \otimes \mathbf{n} - \frac{\mathbb{1}}{3}$, which is characterized by its invariance under $\mathbf{n} \to -\mathbf{n}$. Accordingly, the global order parameter is defined as $\mathbb{Q}[\mathbf{n}] = \langle \mathbb{Q}[\mathbf{n}_i] \rangle$ in the coarse-grained order parameter theory and formally relates to the uniaxial order parameter space $O(3)/D_{\infty h} \simeq S^2/Z_2 \simeq \mathbb{RP}^2$, the real projective plane.

4.1.2 General $3D$ orientational order

The above familiar examples share the key feature of having an $O(2)$ symmetry in the plane perpendicular to the ordering vector, which is why the underlying physics is so apparent: the order parameter is defined by one axis and the rotations in the perpendicular plane are trivial, and the degrees of freedom effectively reduce to 1D objects (the spins and the rods in the above examples).

Nonetheless, for general 3D point-group-symmetric ordering, the order parameter and the coarse grained degrees of freedom form intrinsic 3D objects (Fig. 4.2). To define the 3D orientation one therefore has to depart

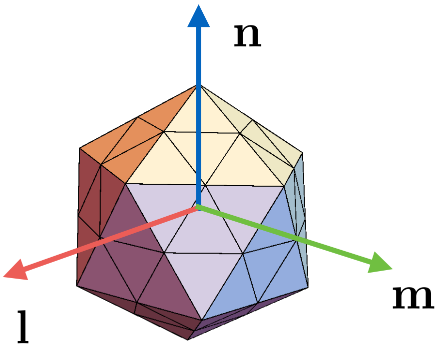

Figure 4.2. To define the orientation of a $3D$ object in general, one need an $O(3)$ triad. Here an icosahedron is used for instance.

from a full $O(3)$ rotation matrix R,

$$R = \begin{pmatrix} \mathbf{l} & \mathbf{m} & \mathbf{n} \end{pmatrix}^T. \tag{4.1}$$

The rows $\{\mathbf{l}, \mathbf{m}, \mathbf{n}\}$ of R form an orthonormal triad $\mathbf{n}^\alpha = \{\mathbf{l}, \mathbf{m}, \mathbf{n}\}$. In other words, R is a rotation that brings the triad $\mathbf{n}^\alpha = \{\mathbf{l}, \mathbf{m}, \mathbf{n}\}$ into coincidence with a fixed "laboratory" frame $\mathbf{e}_a = \{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ and can be defined by three Euler angles with respect to the unit vectors $\mathbf{e}_a$. The determinant of R defines the handedness or chirality of the triad,

$$\sigma = \det R = \epsilon_{abc}(\mathbf{l} \otimes \mathbf{m} \otimes \mathbf{n})_{abc} = \mathbf{l} \cdot (\mathbf{m} \times \mathbf{n}) = \pm 1, \tag{4.2}$$

which is a pseudoscalar and invariant under the proper rotations $SO(3)$. Moreover, due to $O(3) = SO(3) \times \{\mathbb{1}, -\mathbb{1}\}$, we have the decomposition

$$R = \sigma \widetilde{R} = \sigma (\tilde{\mathbf{l}} \quad \widetilde{\mathbf{m}} \quad \tilde{\mathbf{n}})^T \tag{4.3}$$

where $\widetilde{R} \in SO(3)$ and its rows $\tilde{\mathbf{n}}^\alpha = \{\tilde{\mathbf{l}}, \tilde{\mathbf{m}}, \tilde{\mathbf{n}}\}$ are pseudovectors. The $O(3)$ constraints $R^T R = R R^T = \mathbb{1}$ and $\det R = \pm 1$ of course reduce the free parameters to the three Euler angles $\Omega = (\theta, \phi, \varphi)$ and chirality in the frame $\mathbf{e}_a$ but we will find the vector notation with the $O(3)$-constraints understood very useful in the following.

The order parameter has to be invariant under all unbroken point-group transformations. As a result, an orientational order parameter with a point group symmetry G is defined by G-invariant tensors constructed from the triad R or $\mathbf{n}^\alpha = \{\mathbf{l}, \mathbf{m}, \mathbf{n}\}$. These tensors are equivalent to higher order multipoles or (three-dimensional) spherical harmonics. We will denote these order parameters tensors composed of the triads generically as $\mathbb{O}^G$, where the additional label specifies the symmetry group G when appropriate. Concretely, in the two examples in Section 4.1.1, the order parameter tensor is the magnetization vector $\mathbb{O}^{C_{\infty v}}[\mathbf{n}] = \mathbf{n}$ and the second rank tensor or director $\mathbb{O}^{D_{\infty h}}[\mathbf{n}] = \mathbb{Q}[\mathbf{n}]$, respectively. Finally, we note that besides the orientational order, the composite chiral order parameter σ defined in Eq. (4.2) is needed for proper point-group symmetries such as $\{C_n, D_n, T, O, I\}$ due to the breaking of the chiral symmetry of $O(3)$.

As $\mathbb{O}^G$ needs to be uniquely invariant under a given symmetry G, it is in general highly non-trivial to construct its explicit form, even though the polynomial invariants of 3D points groups have been computed a long time ago [94, 95] and the representation theory of $SO(3)$ is known.

4.1.3 Deriving the ordering tensors from the gauge theory

Let us now establish the relation of the ordering tensors with the gauge theory introduced in Chapter 3.1. The goal is to construct a coarse-grained order parameter with certain point group symmetry.

As it has been briefly discussed in Chapter 3.1.3, theunderlying principle of deriving the order parameters is the fundamental gauge theoretical result: all physical observables have to be gauge invariant, since gauge symmetries cannot break spontaneously [28]. By construction, the model Eq. (3.5),

$$H = -\sum_{\langle ij \rangle} \mathrm{Tr}\left[R_i^T \mathbb{J} U_{ij} R_j\right] - \sum_{\square} \sum_{\mathcal{C}_\mu} K_{\mathcal{C}_\mu} \delta_{\mathcal{C}_\mu}(U_\square) \mathrm{Tr}\Big[U_\square\Big], \tag{4.4}$$

embodies the symmetry of the order parameter tensors by the gauge symmetry. In particular, if we integrate out the gauge fields in the Hamiltonian, the terms that survive are gauge invariant local combinations of the matter fields, corresponding to the order parameter tensors. This can be most easily accomplished in the strong coupling limit of the gauge theory $K_{\mathcal{C}} = 0$. In this limit, the gauge theory Eq. (3.5) reduces to

$$H = -\sum_{\langle ij \rangle} \mathrm{Tr}\left[R_i^T \mathbb{J} U_{ij} R_j\right], \tag{4.5}$$

and the gauge fields have no independent dynamics. The result is essentially the effective Hamiltonian of the orientational probability density $\rho(\{R_i\}) \sim \frac{1}{Z} \sum_{\{U_{ij}\}} e^{-\beta H[\{R_i\},\{U_{ij}\}]}$, but in order to find the order parameter tensors we do not need the effective Hamiltonian in closed form and can simply utilize the high-temperature expansion for small β. The couplings $\mathbb{J}$ do not affect the general form of the expansion and we set them to be isotropic $\mathbb{J} = J\mathbb{1}$ for simplicity and measure the temperature in the units $\beta J \equiv \beta$.

The partition function of the model Eq. (4.5) is defined in the usual way,

$$\begin{aligned} Z &= \sum_{\{R_i\}} \sum_{\{U_{ij}\}} e^{-\beta H[R_i, U_{ij}]} \\ &= \sum_{\{\tilde{R}_i\}} \sum_{\{\sigma_i\}} \sum_{\{U_{ij}\}} e^{-\beta H[\tilde{R}_i, \sigma_i, U_{ij}]}, \end{aligned} \tag{4.6}$$

where the summations are naturally discrete over the lattice and discrete or continuous over the groups G and $O(3)$. In the second line we used made the handedness field explicit by Eq. (4.2), $R_i = \sigma_i \widetilde{R}_i$. In order to integrate over the gauge fields, the partition function is Taylor expanded in the high temperature limit $\beta \ll 1$,

$$Z = \sum_{\{\tilde{R}_i\}} \sum_{\{\sigma_i\}} \sum_{\{U_{ij}\}} \prod_{\langle ij \rangle} \sum_{n=0}^{\infty} \frac{1}{n!} (-\beta H_{ij})^n. \tag{4.7}$$

The integration over the gauge fields can be explicitly performed on the lattice order by order in the expansion. By construction, the terms appearing must be local terms that are composed of contractions of gauge invariant tensors. The result is therefore an expression starting with contractions $\sim$ Tr $[\mathbb{O}_i^G \cdot \mathbb{O}_j^G]$ coming from the lowest order non-zero terms $n_{\min} \sim \text{rank } \mathbb{O}^G$ in the expansions. In other words, the lowest order nontrivial terms are composed of the lowest order invariant tensors that can be found from Table 4.1. We emphasize that by construction these tensors are the minimal and simplest possible set of invariant tensors allowed by the symmetries.

4.2 Minimal invariant tensors

4.2.1 Order parameter table

In Table 4.1 we show the lowest order invariant tensors for all the 32 crystallographic point groups, the 2 icosahedral groups and the 5 infinite axial groups.

The standard Schönflies notation [131, 95] is used in Table 4.1. The point groups are defined in the coordinate system spanned by the unit triad vectors $\mathbf{n}^\alpha = \{\mathbf{l}, \mathbf{m}, \mathbf{n}\}$ set up in the following way. All point groups have the origin as their fixed point. The rotational axis of cyclic rotation groups C_n of is chosen to be $\mathbf{n}$. The dihedral group D_n has an additional generator in terms of a π-rotation along the vector $\mathbf{l}$ or $\mathbf{m}$. The group C_{nv} is augmented with a "vertical" reflection in the plane $(\mathbf{l}, \mathbf{n})$. The groups C_{nh} and D_{nh} have an additional "horizontal" reflection plane $(\mathbf{l}, \mathbf{m})$. The group D_{nd} has vertical reflection planes in terms of bisectors of the dihedral π-rotation axes. The groups S_{2n} are composed of n-fold rotations in the plane $\mathbf{l}, \mathbf{m}$. The polyhedral groups T, T_d, T_h and O, O_h are defined in terms of a (tetrahedron embedded) in a cube with face normals $\mathbf{n}^\alpha = \{\mathbf{l}, \mathbf{m}, \mathbf{n}\}$. The group I_h is the symmetry group of an icosahedron with vertices at cyclic permutations of the coordinates $\pm\tau\mathbf{l} \pm \mathbf{m} \pm 0 \cdot \mathbf{n}$ and I its proper subgroup, following the conventions in [132].

Accordingly, $\mathbb{O}^G = \mathbb{O}^G[\mathbf{l}, \mathbf{m}, \mathbf{n}]$ and $\mathbb{O}^G = \{\mathbb{A}^G, \mathbb{B}^G\}$ denote the ordering tensor for polyhedral groups and for axial groups, respectively, where $\mathbb{A}^G = \mathbb{A}^G[\mathbf{n}]$ is the order parameter for the main axis $\mathbf{n}$ and $\mathbb{B}^G = \mathbb{B}^G[\mathbf{l}, \mathbf{m}]$ or $\mathbb{B}^G[\mathbf{l}, \mathbf{m}, \mathbf{n}]$ for the in-plane structure for the finite axial groups. Together with the handedness fields σ, they can uniquely define the order parameter for the symmetries mentioned above.

Amongst the ordering tensors in Table 4.1, the C_1 order parameters $\mathbb{O}^{C_1}[\mathbf{l}, \mathbf{m}, \mathbf{n}] = \{\mathbb{A}^{C_{\infty v}}[\mathbf{n}], \mathbb{B}^{C_1}[\mathbf{l}, \mathbf{m}]\} = \{\mathbf{l}, \mathbf{m}, \mathbf{n}\}$ simply constitute the original $O(3)$-rotor order parameter R of a phase with no unbroken symmetry (C_1 is the trivial group); $\mathbb{O}^{D_{2h}} = \{\mathbb{O}^{D_{\infty h}}[\mathbf{n}], \mathbb{B}^{D_{2h}}[\mathbf{l}, \mathbf{m}]\}$ compose the well known order parameter tensors for D_{2h}-biaxial nematics; $\mathbb{O}^{C_{\infty v}}[\mathbf{n}]$ and $\mathbb{O}^{D_{\infty h}}[\mathbf{n}]$ are the classical Heisenberg spin $\mathbf{n}$ and uniaxial director $\mathbb{Q}[\mathbf{n}]$, respectively; $\mathbb{O}^{O_h}[\mathbf{l}, \mathbf{m}, \mathbf{n}]$ has been discussed in Ref. [18]; $\mathbb{O}^{T_d}[\mathbf{l}, \mathbf{m}, \mathbf{n}]$ and $\mathbb{O}^{I_h}[\mathbf{l}, \mathbf{m}, \mathbf{n}]$ appear in a different form in Ref. [89], where an incomplete classification of order parameters for subgroups of $SO(3)$ is also discussed. However, many of the order parameter tensors in Table 4.1 are new and have not been classified in the context of a single unified framework.

Table 4.1. Classification of order parameters for three dimensional point groups. The first column specifies the symmetries and the second column specifies the type $\{\mathbb{O}, \mathbb{A}, \mathbb{B}\}$ of the order constructed from the $O(3)$ triad $R = (\mathbf{l}, \mathbf{m}, \mathbf{n})^T$. The third column gives the explicit form of ordering tensors in the chosen coordinates. They are traceless and vanish in the isotropic phase. The infinite axial groups $\{C_\infty, C_{\infty v}, C_{\infty h}, D_\infty, D_{\infty h}\}$ require a single ordering tensor, $\mathbb{A}[\mathbf{n}]$, describing the orientation of their primary symmetry axis, chosen to be $\mathbf{n}$; the finite axial groups $\{C_n, C_{nv}, C_{nh}, S_{2n}, D_n, D_{nh}, D_{nd}\}$ require two ordering tensors, $\mathbb{A}[\mathbf{n}]$ and $\mathbb{B}[\mathbf{l}, \mathbf{m}]$ or $\mathbb{B}[\mathbf{l}, \mathbf{m}, \mathbf{n}]$, for their primary axis and perpendicular in-plane structure, respectively; the polyhedral groups $\{T, T_d, T_h, O, O_h, I, I_h\}$, which treat $\{\mathbf{l}, \mathbf{m}, \mathbf{n}\}$ symmetrically, require only one ordering tensor $\mathbb{O}[\mathbf{l}, \mathbf{m}, \mathbf{n}]$. Due to the symmetry hierarchy, many point groups share ordering tensors (see Section 4.2.3). Together with the chiral order parameter $\sigma = \det R = \pm 1$ arisen for proper point groups, these ordering tensors uniquely define the orientational ordering of three dimensional point groups. For example, the order parameters for finite proper axial groups are given by $\mathbb{O}^G = \{\mathbb{A}^G, \mathbb{B}^G, \sigma\}$. ${}^{\otimes n}$ denotes the tensor power, e.g., $\mathbf{n}^{\otimes 2} = \mathbf{n} \otimes \mathbf{n}$ and $\delta_{ab} \bigotimes_{\mu=a,b} \mathbf{e}_\mu = \delta_{ab} \mathbf{e}_a \otimes \mathbf{e}_b$. $\tau = (1+\sqrt{5})/2$ is the golden ratio. $\sum_{\text{cyc}}$ runs over cyclic permutations of $\{\mathbf{l}, \mathbf{m}, \mathbf{n}\}$. $\sum_{\text{perm}}$ sums over all non-equivalent combinations of the indices of the tensor. $\sum_{\text{perm}''}$ in the $\{C_{6v}, D_6, D_{6h}\}$ cases sums over all the six permutations of the indices d, e and f, and $\sum_{\text{perm}'} = \sum_{\text{perm}} - \sum_{\text{perm}''}$. $\sum_{\{+,-\}}$ for the $\{I, I_h\}$ is a sum over the four combinations of the two $\pm$ signs.

Symmetry Groups	Type	Ordering Tensors	Tensor Rank
$C_1,\, C_{1h}$	$\mathbb{B}[\mathbf{l},\mathbf{m}]$	$\mathbf{l},\, \mathbf{m}$	1
S_2	$\mathbb{B}[\mathbf{l},\mathbf{m},\mathbf{n}]$	$\mathbf{l}\otimes\mathbf{m},\, \mathbf{m}\otimes\mathbf{l},\, \mathbf{m}\otimes\mathbf{n},\, \mathbf{n}\otimes\mathbf{m},\, \mathbf{n}\otimes\mathbf{l},\, \mathbf{l}\otimes\mathbf{n}$	2
$C_2,\, C_{2h}$	$\mathbb{B}[\mathbf{l},\mathbf{m}]$	$\mathbf{l}\otimes\mathbf{m},\, \mathbf{m}\otimes\mathbf{l}$	2
$C_{2v},\, D_2,\, D_{2h}$	$\mathbb{B}[\mathbf{l},\mathbf{m}]$	$\mathbf{l}\otimes\mathbf{l} - \frac{1}{3}\mathbb{1},\, \mathbf{m}\otimes\mathbf{m} - \frac{1}{3}\mathbb{1}$	2
S_4	$\mathbb{B}[\mathbf{l},\mathbf{m},\mathbf{n}]$	$\left(\mathbf{l}\otimes\mathbf{l} - \mathbf{m}\otimes\mathbf{m}\right)\otimes\mathbf{n}$	3
D_{2d}	$\mathbb{B}[\mathbf{l},\mathbf{m},\mathbf{n}]$	$\left(\mathbf{l}\otimes\mathbf{m} + \mathbf{m}\otimes\mathbf{l}\right)\otimes\mathbf{n}$	3
$C_3,\, C_{3h}$	$\mathbb{B}[\mathbf{l},\mathbf{m}]$	$\left(\mathbf{l}^{\otimes 3} - \mathbf{l}\otimes\mathbf{m}^{\otimes 2} - \mathbf{m}\otimes\mathbf{l}\otimes\mathbf{m} - \mathbf{m}^{\otimes 2}\otimes\mathbf{l}\right),$ $\left(\mathbf{m}^{\otimes 3} - \mathbf{m}\otimes\mathbf{l}^{\otimes 2} - \mathbf{l}\otimes\mathbf{m}\otimes\mathbf{l} - \mathbf{l}^{\otimes 2}\otimes\mathbf{m}\right)$	3
$C_{3v},\, D_3,\, D_{3h}$	$\mathbb{B}[\mathbf{l},\mathbf{m}]$	$\left(\mathbf{l}^{\otimes 3} - \mathbf{l}\otimes\mathbf{m}^{\otimes 2} - \mathbf{m}\otimes\mathbf{l}\otimes\mathbf{m} - \mathbf{m}^{\otimes 2}\otimes\mathbf{l}\right)$	3
S_6	$\mathbb{B}[\mathbf{l},\mathbf{m},\mathbf{n}]$	$\left(\mathbf{l}^{\otimes 3} - \mathbf{l}\otimes\mathbf{m}^{\otimes 2} - \mathbf{m}\otimes\mathbf{l}\otimes\mathbf{m} - \mathbf{m}^{\otimes 2}\otimes\mathbf{l}\right)\otimes\mathbf{n},$ $\left(\mathbf{m}^{\otimes 3} - \mathbf{m}\otimes\mathbf{l}^{\otimes 2} - \mathbf{l}\otimes\mathbf{m}\otimes\mathbf{l} - \mathbf{l}^{\otimes 2}\otimes\mathbf{m}\right)\otimes\mathbf{n}$	4
D_{3d}	$\mathbb{B}[\mathbf{l},\mathbf{m},\mathbf{n}]$	$\left(\mathbf{m}^{\otimes 3} - \mathbf{m}\otimes\mathbf{l}^{\otimes 2} - \mathbf{l}\otimes\mathbf{m}\otimes\mathbf{l} - \mathbf{l}^{\otimes 2}\otimes\mathbf{m}\right)\otimes\mathbf{n}$	4
$C_4,\, C_{4h}$	$\mathbb{B}[\mathbf{l},\mathbf{m}]$	$\mathbf{l}^{\otimes 3}\otimes\mathbf{m} - \mathbf{m}^{\otimes 3}\otimes\mathbf{l}$	4
$C_{4v},\, D_4,\, D_{4h}$	$\mathbb{B}[\mathbf{l},\mathbf{m}]$	$\mathbf{l}^{\otimes 2}\otimes\mathbf{m}^{\otimes 2} + \mathbf{m}^{\otimes 2}\otimes\mathbf{l}^{\otimes 2} -$ $\frac{4}{15}\delta_{ab}\delta_{cd}\bigotimes_{\mu=a,b,c,d}\mathbf{e}_\mu +$ $\frac{1}{15}\left(\delta_{ac}\delta_{bd}\bigotimes_{\mu=a,c,b,d}\mathbf{e}_\mu + \delta_{ad}\delta_{bc}\bigotimes_{\mu=a,d,b,c}\mathbf{e}_\mu\right),$ $\mathbf{l}^{\otimes 4} + \mathbf{m}^{\otimes 4} - \frac{2}{15}\sum_{\text{perm}}\delta_{ab}\delta_{cd}\bigotimes_{\mu=a,b,c,d}\mathbf{e}_\mu$	4
$C_6,\, C_{6h}$	$\mathbb{B}[\mathbf{l},\mathbf{m}]$	$\left(\mathbf{l}^{\otimes 3} - \mathbf{l}\otimes\mathbf{m}^{\otimes 2} - \mathbf{m}\otimes\mathbf{l}\otimes\mathbf{m} - \mathbf{m}^{\otimes 2}\otimes\mathbf{l}\right)\otimes$ $\left(\mathbf{m}^{\otimes 3} - \mathbf{m}\otimes\mathbf{l}^{\otimes 2} - \mathbf{l}\otimes\mathbf{m}\otimes\mathbf{l} - \mathbf{l}^{\otimes 2}\otimes\mathbf{m}\right),$ $\left(\mathbf{m}^{\otimes 3} - \mathbf{m}\otimes\mathbf{l}^{\otimes 2} - \mathbf{l}\otimes\mathbf{m}\otimes\mathbf{l} - \mathbf{l}^{\otimes 2}\otimes\mathbf{m}\right)\otimes$ $\left(\mathbf{l}^{\otimes 3} - \mathbf{l}\otimes\mathbf{m}^{\otimes 2} - \mathbf{m}\otimes\mathbf{l}\otimes\mathbf{m} - \mathbf{m}^{\otimes 2}\otimes\mathbf{l}\right)$	6
$C_{6v},\, D_6,\, D_{6h}$	$\mathbb{B}[\mathbf{l},\mathbf{m}]$	$\left(\mathbf{l}^{\otimes 3} - \mathbf{l}\otimes\mathbf{m}^{\otimes 2} - \mathbf{m}\otimes\mathbf{l}\otimes\mathbf{m} - \mathbf{m}^{\otimes 2}\otimes\mathbf{l}\right)^{\otimes 2} +$ $\frac{4}{105}\sum_{\text{perm}'}\delta_{ab}\delta_{cd}\delta_{ef}\bigotimes_{\substack{\mu=a,b,c,\\ d,e,f}}\mathbf{e}_\mu -$ $\frac{2}{21}\sum_{\text{perm}''}\delta_{ad}\delta_{be}\delta_{cf}\bigotimes_{\substack{\mu=a,d,b,\\ e,c,f}}\mathbf{e}_\mu,$ $\left(\mathbf{m}^{\otimes 3} - \mathbf{m}\otimes\mathbf{l}^{\otimes 2} - \mathbf{l}\otimes\mathbf{m}\otimes\mathbf{l} - \mathbf{l}^{\otimes 2}\otimes\mathbf{m}\right)^{\otimes 2} +$ $\frac{4}{105}\sum_{\text{perm}'}\delta_{ab}\delta_{cd}\delta_{ef}\bigotimes_{\substack{\mu=a,b,c,\\ d,e,f}}\mathbf{e}_\mu -$ $\frac{2}{21}\sum_{\text{perm}''}\delta_{ad}\delta_{be}\delta_{cf}\bigotimes_{\substack{\mu=a,d,b,\\ e,c,f}}\mathbf{e}_\mu$	6
$C_n, C_{nv},\, C_\infty, C_{\infty v}$	$\mathbb{A}[\mathbf{n}]$	$\mathbf{n}$	1
$C_{\infty h}$	$\mathbb{A}[\mathbf{n}]$	$\sigma\mathbf{n}$	1
$S_{2n}, C_{nh}, D_n,$ $D_{nh}, D_{nd}, D_\infty,\, D_{\infty h}$	$\mathbb{A}[\mathbf{n}]$	$\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathbb{1}$	2
T	$\mathbb{O}[\mathbf{l},\mathbf{m},\mathbf{n}]$	$\sum_{\text{cyc}}\mathbf{l}\otimes\mathbf{m}\otimes\mathbf{n}$	3
T_d	$\mathbb{O}[\mathbf{l},\mathbf{m},\mathbf{n}]$	$\sum_{\text{cyc}}\left(\mathbf{l}\otimes\mathbf{m} + \mathbf{m}\otimes\mathbf{l}\right)\otimes\mathbf{n}$	3
T_h	$\mathbb{O}[\mathbf{l},\mathbf{m},\mathbf{n}]$	$\mathbf{m}^{\otimes 2}\otimes\mathbf{l}^{\otimes 2} + \mathbf{l}^{\otimes 2}\otimes\mathbf{n}^{\otimes 2} + \mathbf{n}^{\otimes 2}\otimes\mathbf{m}^{\otimes 2} -$ $\frac{2}{5}\delta_{ab}\delta_{cd}\bigotimes_{\mu=a,b,c,d}\mathbf{e}_\mu + \frac{1}{10}\Big(\delta_{ac}\delta_{bd}\bigotimes_{\mu=a,c,b,d}\mathbf{e}_\mu +$ $\delta_{ad}\delta_{bc}\bigotimes_{\mu=a,d,b,c}\mathbf{e}_\mu\Big)$	4
$O,\, O_h$	$\mathbb{O}[\mathbf{l},\mathbf{m},\mathbf{n}]$	$\mathbf{l}^{\otimes 4} + \mathbf{m}^{\otimes 4} + \mathbf{n}^{\otimes 4} - \frac{1}{5}\sum_{\text{perm}}\delta_{ab}\delta_{cd}\bigotimes_{\mu=a,b,c,d}\mathbf{e}_\mu$	4
$I,\, I_h$	$\mathbb{O}[\mathbf{l},\mathbf{m},\mathbf{n}]$	$\sum_{\text{cyc}}\left[\mathbf{l}^{\otimes 6} + \sum_{\{+,-\}}\left(\frac{1}{2}\mathbf{l} \pm \frac{\tau}{2}\mathbf{m} \pm \frac{1}{2\tau}\mathbf{n}\right)^{\otimes 6}\right] -$ $\frac{1}{7}\sum_{\text{perm}}\delta_{ab}\delta_{cd}\delta_{ef}\bigotimes_{\substack{\mu=a,b,c,\\ d,e,f}}\mathbf{e}_\mu$	6

4.2.2 Structure of the ordering tensors

Continuous axial groups

The five infinite axial groups $\{C_\infty, C_{\infty v}, C_{\infty h}, D_\infty, D_{\infty h}\}$ require only one tensor to define the associated orientational order. This is because these groups contain a plane perpendicular to the vector $\mathbf{n}$ with continuous $SO(2)$ or $O(2)$ rotations, hence their in-plane structure is trivial and the order parameter effectively reduces to a vector $(C_\infty, C_{\infty v})$, a pseudovector $(C_{\infty h})$ or a director $(D_\infty, D_{\infty h})$, up to an additional chiral order parameter σ for the proper point groups.

Finite axial groups

Finite axial groups $\{C_n, C_{nv}, S_{2n}, C_{nh}, D_n, D_{nh}, D_{nd}\}$ require two ordering tensors $\{\mathbb{A}, \mathbb{B}\}$: $\mathbb{A} = \mathbb{A}[\mathbf{n}]$ describes the orientation of the primary axis, which is always chosen as $\mathbf{n}$ in Table 4.1, and tensors $\mathbb{B} = \mathbb{B}[\mathbf{l}, \mathbf{m}]$ or $\mathbb{B}[\mathbf{l}, \mathbf{m}, \mathbf{n}]$ for the perpendicular in-plane order. This generalizes well-known structure of the order parameters of biaxial (D_{2h}) liquid crystals. Due to symmetry relations which will be discussed later, the primary ordering tensors $\mathbb{A}[\mathbf{n}]$ for $\{C_n, C_{nv},\}$ and $\{S_{2n}, C_{nh}, D_n, D_{nh}, D_{nd}\}$ are identical to the order parameters $\mathbb{O}^{C_{\infty v}}[\mathbf{n}]$ and $\mathbb{O}^{D_{\infty h}}[\mathbf{n}]$, respectively.

Polyhedral groups

The finite symmetry groups $\{T, T_d, T_h, O, O_h, I, I_h\}$ related to the regular tetrahedron, octahedron and icosahedron, respectively, require only one ordering tensor involving the whole triad $\mathbf{n}^\alpha$. These symmetries permute $\{\mathbf{l}, \mathbf{m}, \mathbf{n}\}$ "isotropically" amongst each other, so there is no primary axis and the three axes appear symmetrically in the order parameter tensor.

Proper point groups: chirality

Besides the orientational order parameters, the proper point group symmetries $\{C_n, D_n, T, O, I\}$ are chiral and have an additional chiral order parameter. The simplest chiral order parameter is just the pseudoscalar handedness or chirality σ of the triad defined in Eq. (4.2). By definition, proper point groups do not possess any inversions and reflections and therefore cannot change the chirality or handedness of the triad.

4.2.3 Point groups and ordering tensors

As one may have already noticed from the above discussion and Table 4.1, although a symmetry can be uniquely defined by the collection of order parameter tensors $\mathbb{O}^G$ and the handedness σ, owing to the group structure, many orientational ordering tensors are shared by different symmetries. We will now clarify this by discussing their group structures.

Firstly, the primary ordering tensor $\mathbb{A}^G[\mathbf{n}]$ for C_n and C_{nv} groups is just the order parameter tensor of the C_∞ and $C_{\infty v}$ groups, $\mathbb{A}^{C_n}[\mathbf{n}] = \mathbb{A}^{C_v}[\mathbf{n}] = \mathbb{O}^{C_\infty}[\mathbf{n}] = \mathbb{O}^{C_{\infty v}}[\mathbf{n}]$. This is due to the simple fact that C_n and C_{nv} groups do not transform $\mathbf{n}$, hence they differ from C_∞ and $C_{\infty v}$ only by their in-plane structure related to $\mathbb{B}^G[\mathbf{l}, \mathbf{m}]$. Similarly, the groups $\{S_{2n}, C_{nh}, D_n, D_{nh}, D_{nd}\}$ have the same effect on $\mathbf{n}$, $\mathbf{n} \to -\mathbf{n}$. Therefore, neglecting the $\mathbf{l}$ and $\mathbf{m}$ components, these symmetries lead to the same primary ordering tensor $\mathbb{A}[\mathbf{n}] = \mathbb{Q}[\mathbf{n}]$, the uniaxial director.

Moreover, the groups $\{C_n, C_{nh}, C_{nv}, D_n, D_{nh}\}$ are closely related in terms of symmetries. C_n and $C_{nh} = C_n \times \{\mathbb{1}, \sigma_h\}$ only differ by a reflection $\sigma_h : \mathbf{n} \to -\mathbf{n}$ in the horizontal mirror $(\mathbf{l}, \mathbf{m})$-plane perpendicular to $\mathbf{n}$. Thus C_n and C_{nh} have the same in-plane structure leading to the same secondary order parameter $\mathbb{B}^{C_n}[\mathbf{l}, \mathbf{m}]$. For the point groups $\{C_{nv}, D_n, D_{nh}\}$, we have $D_{nh} = D_n \times \{\mathbb{1}, \sigma_h\}$ and C_{nv} and D_n can be represented as semi-direct products $C_{nv} = C_n \rtimes \{\mathbb{1}, \sigma_v\}$ and $D_n = C_n \rtimes \{\mathbb{1}, c_2(\mathbf{l})\}$, where σ_v is a reflection $(\mathbf{l}$,$\mathbf{n})$-plane and $c_2(\mathbf{l})$ is a two-fold rotation around the axis $\mathbf{l}$,

$$\sigma_v = \sigma_{\mathbf{ln}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad c_2(\mathbf{l}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{4.8}$$

It is immediately clear that, σ_v and $c_2(\mathbf{l})$ have the same action on the $\mathbf{l}$ and $\mathbf{m}$ components. Therefore, $\{C_{nv}, D_n, D_{nh}\}$ also have the same in-plane order parameter $\mathbb{B}[\mathbf{l}, \mathbf{m}]$.

The common structures of the finite axial groups have a direct implication on the associated phase transitions. For a phase with the symmetry of a finite axial group, it is in principle possible to disorder the primary and secondary order separately before the transition to the isotropic phase. If we first disorder the secondary order in a plane, the following sequences of phase transitions can happen

$$
\begin{aligned}
&C_n, C_{nv} \to C_{\infty v} \to O(3), \\
&S_{2n}, C_{nh}, D_n, D_{nh}, D_{nd} \to D_{\infty h} \to O(3),
\end{aligned} \tag{4.9}
$$

related to the restoration of the in-plane $O(2)$ symmetry followed by disordering of order along the principal axis $\mathbf{n}$. These transitions generalize the biaxial-uniaxial-isotropic liquid transition of biaxial liquid crystals [72, 71]. We have numerically verified the transition sequences in Eq. (4.9) for a large number of symmetries and will present the detailed analyses for their phase diagrams in the next chapter.

Finally, in the case of the polyhedral groups, $T_h = T \times \{\mathbb{1}, -\mathbb{1}\}$, $O_h = O \times \{\mathbb{1}, -\mathbb{1}\}$ and $I_h = I \times \{\mathbb{1}, -\mathbb{1}\}$ are generated from the proper subgroups T, O and I by adding the inversion $-\mathbb{1}$. Since the ordering tensors of I and O in Table 4.1 are of even rank, this difference is not reflected directly in the orientational order parameters. There exist higher order invariant tensors that can distinguish O (I) from O_h (I_h), nonetheless one needs to consider at least a rank-5 (rank-7) tensors and it is therefore more convenient to distinguish them by the chirality σ (see Section 4.3.3 for more details).

Improper groups possessing only reflections but not the inversions $-\mathbb{1}$, including all axial groups C_{nv} for all n, $\{S_{2n}, C_{nh}, D_{nh}\}$ for odd n, D_{nd} for even n and the regular tetrahedral group T_d, have non-vanishing odd-rank order parameters in general. In these order parameters, terms related with right and left handed triads appear equally, making the order parameter invariant under certain improper reflections but not inversions. This will be reflected in the structure of the associated order parameters. For instance, as can be seen from Table 4.1, the order parameter for the tetrahedral-T_d group, $\mathbb{O}^{T_d}$ consists of a left and right handed copy of that of the tetrahedral-T group (see Section 4.3.3 for more details).

4.2.4 Determining the symmetry of a phase and phase transitions with ordering tensors

The ordering tensors we show in Table 4.1 generalize the local director tensor $\mathbb{Q}_{ab}$ for uniaxial nematics. The macroscopic order parameters are defined as coarse grained averages over the system

$$
\langle \mathbb{O}^G \rangle = \frac{1}{V} \sum_i \langle \mathbb{O}_i^G \rangle, \tag{4.10}
$$

where V denotes the spatial averaging volume. To verify the symmetry of a phase, one need in principle consider all independent entries of the order parameter tensor. This is in general quite involved since the number of the entries grows exponentially with the rank of the tensor.

However, for interactions favoring homogeneous a nematic order, such as the interaction in the gauge model Eq. (4.5), the symmetry of the phase can be revealed by the scalar two point functions in the limit of large separation. Since $\langle \mathbb{O}_i^G \rangle$ will develop a finite value in the ordered phase, at long distances the scalar two point function of the order parameter tensor behaves as

$$\begin{aligned} &\lim_{|i-j|\to\infty} \langle (\mathbb{O}_i^G)_{abc\ldots} (\mathbb{O}_j^G)_{abc\ldots} \rangle \\ &= \begin{cases} \mathrm{Tr}\ \langle \mathbb{O}_i^G \rangle^2 > 0 & \text{nematic} \\ 0 & \text{otherwise.} \end{cases} \end{aligned} \tag{4.11}$$

The contractions in Tr $(\bullet)$ are determined up to the tensor symmetries of the order parameter. This allows us to define a strength for the ordering tensors,

$$q = \sqrt{\langle (\mathbb{O}_i^G)_{abc\ldots} \rangle^2}, \tag{4.12}$$

and the symmetry of the phase can be defined by the lowest order tensor and "smallest" group G with $q \neq 0$. Accordingly, a phase transition associated with $\langle \mathbb{O}_i^G \rangle$ can be identified from the susceptibility $\chi(q)$ of the ordering strength,

$$\chi(q) = \beta V \Big(\langle q^2 \rangle - \langle q \rangle^2 \Big). \tag{4.13}$$

We have numerically computed q and $\chi(q)$ in the model Eq. (4.5) for large number of point group symmetries [23]. Our simulations showed that $\chi(q)$ will exhibit a clear peak at the temperature where the heat capacity peaks, indicating that q in combination of simple symmetry arguments is indeed sufficient to determine the symmetry of a nematic phase with homogeneous distribution of order parameters.

However, we note that, when non-homogeneous distributions of order parameters are preferred, the symmetry of a state can be compatible but not identical to G, as also discussed, e.g., in Ref. [92]. In these cases, a non-zero q is not sufficient to identify the symmetry of the state, and one in principle need consider all components of $\langle \mathbb{O}_i^G \rangle$. However, the symmetry of a phase may be also determined by the "eigenvalues" and the distribution of non-zero entries of $\langle \mathbb{O}_i^G \rangle$ [133]. Studies with this regard so far mostly concentrate on the rank-2 $D_{\infty h}$ and D_{2h} ordering tensors [134–136, 120]; it would be interesting to consider the ordering of the tensors in Table 4.1 in full generality without assumptions on microscopic configurations of a particular model.

4.3 Examples and discussion

In this section we will discuss some concrete examples of deriving the order parameter tensors in Table 4.1. For all finite and discrete point groups, we can integrate over the gauge fields in the expansion Eq. (4.7). For the continuous axial groups, we can do the integrations in closed form. The results are by construction composed of local contractions of the simplest gauge invariant tensors allowed by the symmetries, i.e. the tensors in Table 4.1.

4.3.1 Continuous axial groups: unixial nematics

The integration over the gauge groups $\{C_\infty, C_{\infty v}, C_{\infty h}, D_\infty, D_{\infty h}\}$ will lead to the familiar results. We will use the D_∞-uniaxial nematic as an example of the general procedure of deriving uniaxial nematic order parameters, the others being similar. The key point is the elimination of the triad vectors $\mathbf{l}, \mathbf{m}$ in the plane where the $SO(2)$-symmetry acts from the Hamiltonian upon integrating out the $SO(2)$-gauge fields, since there can be no gauge invariant combinations of these components in any finite order.

The gauge fields $U_{ij} \in D_\infty$ can be generated by the transformations $\{c_\theta(\mathbf{n}), c_2(\mathbf{m})\}$, where

$$c_\theta(\mathbf{n}) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}, c_2(\mathbf{m}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{4.14}$$

are a rotation about $\mathbf{n}$ by an angle $\theta \in [0, 2\pi)$ and a π-rotation about $\mathbf{m}$, respectively. We note that the "usual" uniaxial symmetry is given by $D_{\infty h} = D_\infty \times \{\mathbb{1}, -\mathbb{1}\}$ and follows with minimal modifications. We focus on the terms in the $(\mathbf{l}, \mathbf{m})$-plane and parametrize the gauge transformation as

$$U_{ij} = \begin{pmatrix} \sigma_{11}\cos\theta_{ij} & \sigma_{12}\sin\theta_{ij} & \\ -\sigma_{21}\sin\theta_{ij} & \sigma_{22}\cos\theta_{ij} & \\ & & \sigma_{33} \end{pmatrix} \in D_\infty, \tag{4.15}$$

where $\theta_{ij} \in [0, 2\pi)$ parametrizes the C_∞ rotation and the constrained signs $\sigma_{\alpha\beta} = \pm 1$ are determined by the presence of the π-rotation in the orthogonal $(\mathbf{l}, \mathbf{n})$-plane. This gives from Eq. (4.5), with $\mathbb{J} = J\mathbb{1}$,

$$\begin{aligned} & H[\mathbf{l}, \mathbf{m}, \mathbf{n}, \theta, \sigma_{\alpha\beta}] \\ & = \sum_{\langle ij \rangle} \Big[\cos\theta_{ij}\Big(\sigma_{11}\mathbf{l}_i \cdot \mathbf{l}_j + \sigma_{22}\mathbf{m}_i \cdot \mathbf{m}_j\Big) \\ & \quad + \sin\theta_{ij}\Big(\sigma_{12}\mathbf{l}_i \cdot \mathbf{m}_j - \sigma_{21}\mathbf{m}_i \cdot \mathbf{l}_j\Big) + \mathbf{n}_i U_{ij,33} \cdot \mathbf{n}_j \Big]. \end{aligned} \tag{4.16}$$

Now we proceed to integrate over the $SO(2)$ angle θ_{ij}

$$\begin{aligned} & e^{-\beta H_{\text{eff}}[\mathbf{l}_i, \mathbf{l}_j, \mathbf{m}_i, \mathbf{m}_j, \sigma_{\alpha\beta}]} \\ & = \prod_{\langle ij \rangle} \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\theta_{ij}\ e^{-H[\mathbf{l}_i, \mathbf{l}_j, \mathbf{m}_i, \mathbf{m}_j, \theta_{ij}, \sigma_{\alpha\beta}]} \\ & = \prod_{\langle ij \rangle} I_0(J_1\sqrt{A_{ij}^2 + B_{ij}^2}). \end{aligned} \tag{4.17}$$

where $I_0(z)$ is a Bessel function of the first kind with the argument

$$\begin{aligned} & A_{ij}^2 + B_{ij}^2 \\ & = \Big[\sigma_{11}\mathbf{l}(i) \cdot \mathbf{l}(j) + \sigma_{22}\mathbf{m}(i) \cdot \mathbf{m}(j)\Big]^2 + \Big[\sigma_{12}\mathbf{l}(i) \cdot \mathbf{m}(j) - \sigma_{21}\mathbf{m}(i) \cdot \mathbf{l}(j)\Big]^2 \\ & = (\mathbf{l}_i \cdot \mathbf{l}_j)^2 + (\mathbf{m}_i \cdot \mathbf{m}_j)^2 + (\mathbf{m}_i \cdot \mathbf{l}_j)^2 + (\mathbf{l}_i \cdot \mathbf{m}_j)^2 \\ & \qquad + 2\sigma_{11}\sigma_{22}(\mathbf{m}_i \cdot \mathbf{m}_j)(\mathbf{l}_i \cdot \mathbf{l}_j) - 2\sigma_{12}\sigma_{21}(\mathbf{l}_i \cdot \mathbf{m}_j)(\mathbf{m}_i \cdot \mathbf{l}_j). \end{aligned} \tag{4.18}$$

Now, since $\det_{2\times 2} U_{ij} = \sigma_{11}\sigma_{22}\cos^2\theta_{ij} + \sigma_{12}\sigma_{21}\sin^2\theta_{ij} = \pm 1 = \det U_{ij} \times$

$U_{33,ij}$, we can simplify

$$
\begin{aligned}
&A_{ij}^2 + B_{ij}^2 \\
&= (\mathbf{l}_i \cdot \mathbf{l}_j)^2 + (\mathbf{m}_i \cdot \mathbf{m}_j)^2 + (\mathbf{m}_i \cdot \mathbf{l}_j)^2 + (\mathbf{l}_i \cdot \mathbf{m}_j)^2 \\
&\quad + 2 \det_{2\times 2} U_{ij} \Big[(\mathbf{m}_i \cdot \mathbf{m}_j)(\mathbf{l}_i \cdot \mathbf{l}_j) - (\mathbf{l}_i \cdot \mathbf{m}_j)(\mathbf{m}_i \cdot \mathbf{l}_j) \Big] \\
&= 1 + (\mathbf{n}_i \cdot \mathbf{n}_j)^2 + 2 \det_{2\times 2} U_{ij} \sigma_i \sigma_j \mathbf{n}_i \cdot \mathbf{n}_j \\
&= (\sigma_i \sigma_j \mathbf{n}_i \cdot \mathbf{n}_j + \det_{2\times 2} U_{ij})^2,
\end{aligned}
\tag{4.19}
$$

where on the second-to-last line we used the $O(3)$ relation $\mathbf{l}_i \times \mathbf{m}_i = \sigma_i \mathbf{n}_i$. Using $\det_{2\times 2} U_{ij} = U_{ij,33}$ gives the result

$$
H_{\text{eff}}[\mathbf{n}_i, U_{ij}] = -\sum_{\langle ij \rangle} \beta \mathbf{n}_i \cdot U_{ij,33} \mathbf{n}_j + \log I_0 \Big(\beta |\sigma_i \sigma_j \mathbf{n}_i \cdot \mathbf{n}_j + U_{ij,33}| \Big),
\tag{4.20}
$$

where $U_{ij,33} = \pm 1 \in Z_2$ since for $U_{ij} \in D_\infty / C_\infty \simeq \{\mathbb{1}, c_2(\mathbf{m})\} = Z_2$ when acting on $\mathbf{n}_i$. We recall that

$$
I_0(z) = \sum_{k=0}^{\infty} \frac{(z^2/4)^k}{(k!)^2},
\tag{4.21}
$$

meaning that to lowest order in β, we generate the term

$$
\begin{aligned}
&\delta H_{\text{eff}}[\mathbf{n}_i, U_{ij,33}] \\
&\sim \sum_{\langle ij \rangle} \frac{\beta^2}{4} \Big[1 + 2\sigma_i \sigma_j \mathbf{n}_i \cdot U_{ij,33} \mathbf{n}_j + (\mathbf{n}_i \cdot \mathbf{n}_j)^2 \Big] + O(\beta^4) \\
&\sim \sum_{\langle ij \rangle} \frac{\beta^2}{2} \tilde{\mathbf{n}}_i U_{ij,33} \cdot \tilde{\mathbf{n}}_j + \text{higher orders},
\end{aligned}
\tag{4.22}
$$

in addition to the original Hamiltonian in terms of $\mathbf{n}_i$. By integrating out $U_{ij,33} \in Z_2$ one will find that all odd powers of $\mathbf{n}_i \cdot \mathbf{n}_j$ vanish and the first non-trivial term is second order with D_∞-invariant scalar contractions

$$
(\tilde{\mathbf{n}}_i \cdot \tilde{\mathbf{n}}_j)^2 = (\mathbf{n}_i \cdot \mathbf{n}_j)^2 = \text{Tr}[\mathbb{Q}_i \cdot \mathbb{Q}_j] + \mathit{const.},
\tag{4.23}
$$

due to the fact that a pseudovector and a vector are indistinguishable for even powers. At the same time, this is the minimal $D_{\infty h}$-invariant tensor contraction $\mathrm{Tr}[\mathbb{Q}_i \cdot \mathbb{Q}_j]$. Higher order terms in Eq. (4.7) are high order even functions such as $[(\mathbf{n}_i \cdot \mathbf{n}_j)^2]^2$, $[(\mathbf{n}_i \cdot \mathbf{n}_j)^2]^3$ etc. that can be neglected as irrelevant. Note however, that the full expansion Eq. (4.7) for D_∞ contains odd powers of β with terms of the form $\beta^3 \sigma_i \sigma_j [(\mathbf{n}_i \cdot \mathbf{n}_j)^2 + \cdots]$ that feature the chiral order parameter σ_i. These chiral terms vanish identically for the case $D_{\infty h}$ when summing over the gauge fields $U_{ij} = \{\mathbb{1}, -\mathbb{1}\}$ in $D_{\infty h} = D_\infty \times \{\mathbb{1}, -\mathbb{1}\}$.

4.3.2 Biaxial nematics

The D_∞- and $D_{\infty h}$-uniaxial nematics we just discussed are a well-known and relatively simple case in the generalized nematic family. Since the symmetries $\{C_\infty, C_{\infty v}, C_{\infty h}, D_\infty, D_{\infty h}\}$ all contain a $SO(2)$ part in the plane perpendicular to the $\mathbf{n}$, the vectors $\mathbf{l}$ and $\mathbf{m}$ disappear from the order parameter, as we saw above. For the symmetries $\{C_n, C_{nv}, C_{nh}, S_{2n}, D_n, D_{nh}, D_{nd}\}$ with finite n, however, there will be in-plane rotational symmetry breaking and we need a secondary "biaxial" order parameter $\mathbb{B}[\mathbf{l}, \mathbf{m}]$ or $\mathbb{B}[\mathbf{l}, \mathbf{m}, \mathbf{n}]$ to capture these phase transitions.

D_{2h}-biaxial order parameter

As can be seen from Table 4.1, for some axial nematics, there exist more than one biaxial order parameters $\mathbb{B}$. A familiar example is the biaxial D_{2h}-nematic, where we have the order parameters $\{\mathbb{B}_1^{D_{2h}}, \mathbb{B}_2^{D_{2h}}\}$,

$$\mathbb{B}_1^{D_{2h}} = \mathbf{l} \otimes \mathbf{l} - \frac{\mathbb{1}}{3}, \tag{4.24a}$$

$$\mathbb{B}_2^{D_{2h}} = \mathbf{m} \otimes \mathbf{m} - \frac{\mathbb{1}}{3} \tag{4.24b}$$

which are both clearly invariant under D_2 generated by $\{c_2(\mathbf{n}), c_2(\mathbf{l})\}$ and as well as the inversion $-\mathbb{1}$. Correspondingly, when integrating over $U_{ij} \in D_{2h}$ in the expansion Eq. (4.7), in the first non-trivial order one will obtain the scalar contractions

$$\begin{aligned} &\sim (l_a l_b)_i (l_a l_b)_j + (m_a m_b)_i (m_a m_b)_j + (n_a n_b)_i (n_a n_b)_j \\ &= \mathrm{Tr}[\mathbb{Q} \cdot \mathbb{Q}] + \mathrm{Tr}[\mathbb{B}_1^{D_{2h}} \cdot \mathbb{B}_1^{D_{2h}}] + \mathrm{Tr}[\mathbb{B}_2^{D_{2h}} \cdot \mathbb{B}_2^{D_{2h}}] + const., \end{aligned} \tag{4.25}$$

which cannot be written as a contraction a single local quantity like in Eq. (4.23). However, due to the $O(3)$-constraint,

$$\mathbf{l} \otimes \mathbf{l} + \mathbf{m} \otimes \mathbf{m} + \mathbf{n} \otimes \mathbf{n} = \mathbb{1}, \tag{4.26}$$

the commonly used D_{2h} biaxial order parameter tensor $\mathbb{B} = \mathbf{l}\otimes\mathbf{l} - \mathbf{m}\otimes\mathbf{m}$ is just a linear combination of $\{\mathbb{B}_1^{D_{2h}}, \mathbb{B}_2^{D_{2h}}\}$ and Eq. (4.25) reduces to contractions of the two independent rank-2 tensors.

Generalized biaxial order parameters

To show how more complicated order parameters are derived using the gauge theory, we next discuss the derivation of the secondary in-plane order parameters $\mathbb{B}^G$ of higher rank using the the order parameters of D_{2d}, D_{4h} and C_{6h} symmetries as examples.

We take D_{2d} symmetry as an example of a nematic with a third-rank order parameter. The D_{2d} group is generated by $\{c_2(\mathbf{n}), c_2(\mathbf{m}), \sigma_d\}$, where

$$c_2(\mathbf{n}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \sigma_d = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{4.27}$$

are a 2-fold rotation about $\mathbf{n}$ and a reflection about the $(\mathbf{l}+\mathbf{m}, \mathbf{n})$ plane and $c_2(\mathbf{m})$ is as that in Eq. (4.14).

These lead to a 4-fold symmetry in the $(\mathbf{l}, \mathbf{m})$-plane. To obtain the order parameter describing this symmetry breaking, we follow the same procedure discussed in the previous section, but now the gauge fields U_{ij} in Eq. (4.7) are elements of D_{2d}. Integrating over $U_{ij} \in D_{2d}$, one will find that the first non-trivial order is the second order with a term $(\mathbf{n}_i \cdot \mathbf{n}_j)^2$, which indicates as expected that $\mathbb{Q}[\mathbf{n}]$ is as well an order parameter for D_{2d} nematics. The 4-fold rotational symmetry combined with the reflections starts showing up at the third order in Eq. (4.7), where one finds the following contractions up to a constant factor

$$\begin{aligned} &\sim \sigma_i\sigma_j \Big[(\tilde{\mathbf{l}}_i \cdot \tilde{\mathbf{m}}_j)(\tilde{\mathbf{m}}_i \cdot \tilde{\mathbf{l}}_j) + (\tilde{\mathbf{l}}_i \cdot \tilde{\mathbf{l}}_j)(\tilde{\mathbf{m}}_i \cdot \tilde{\mathbf{m}}_j)\Big](\tilde{\mathbf{n}}_i \cdot \tilde{\mathbf{n}}_j) \\ &= [(l_a m_b + m_a l_b)n_c]_i[(l_a m_b + m_a l_b)n_c]_j \\ &= \mathrm{Tr}\left[\Big[(\mathbf{l}\otimes\mathbf{m} + \mathbf{m}\otimes\mathbf{l})\otimes\mathbf{n}\Big]_i \cdot \Big[(\mathbf{l}\otimes\mathbf{m} + \mathbf{m}\otimes\mathbf{l})\otimes\mathbf{n}\Big]_j\right], \end{aligned} \tag{4.28}$$

where the third-rank contraction $\mathrm{Tr}(\bullet_{abc} \cdot \bullet_{abc})$ is determined up to the symmetries of the order parameter tensor (symmetric in the first two indices). By construction, the local quantity appeared in Eq. (4.28) is D_{2d} invariant, hence can be used to define a D_{2d}-biaxial order parameter,

$$\mathbb{B}^{D_{2d}} = (\mathbf{l}\otimes\mathbf{m} + \mathbf{m}\otimes\mathbf{l})\otimes\mathbf{n}. \tag{4.29}$$

The full order parameter of a D_{2d} nematic is therefore given by

$$\mathbb{O}^{D_{2d}}[\mathbf{l},\mathbf{m},\mathbf{n}] = \{\mathbb{A}^{D_{\infty h}}[\mathbf{n}], \mathbb{B}^{D_{2d}}[\mathbf{l},\mathbf{m},\mathbf{n}]\}. \tag{4.30}$$

Continuing to D_{4h} symmetry, after integrating out the gauge fields for D_{4h}, at the fourth order one will find the following contractions up to constant factors and terms solely depending on the axial axis $\mathbf{n}$,

$$\begin{aligned}\sim \mathrm{Tr}\Big[&(\mathbf{l}_i^{\otimes 4}+\mathbf{m}_i^{\otimes 4})\cdot(\mathbf{l}_j^{\otimes 4}+\mathbf{m}_j^{\otimes 4})+3(\mathbf{l}_i^{\otimes 2}\otimes\mathbf{m}_i^{\otimes 2}\\ &+\mathbf{m}_i^{\otimes 2}\otimes\mathbf{l}_i^{\otimes 2})\cdot(\mathbf{l}_j^{\otimes 2}\otimes\mathbf{m}_j^{\otimes 2}+\mathbf{m}_j^{\otimes 2}\otimes\mathbf{l}_j^{\otimes 2})\Big].\end{aligned} \tag{4.31}$$

One can therefore recognize two D_{4h}-invariant local tensors,

$$\begin{aligned}\mathbb{B}_1^{D_{4h}} &= \mathbf{l}^{\otimes 2}\otimes\mathbf{m}^{\otimes 2}+\mathbf{m}^{\otimes 2}\otimes\mathbf{l}^{\otimes 2}-\frac{4}{15}\delta_{ab}\delta_{cd}\bigotimes_{\mu=a,b,c,d}\mathbf{e}_\mu\\ &\quad+\frac{1}{15}\Big(\delta_{ac}\delta_{bd}\bigotimes_{\mu=a,c,b,d}\mathbf{e}_\mu+\delta_{ad}\delta_{bc}\bigotimes_{\mu=a,d,b,c}\mathbf{e}_\mu\Big),\end{aligned} \tag{4.32}$$

$$\mathbb{B}_2^{D_{4h}} = \mathbf{l}^{\otimes 4}+\mathbf{m}^{\otimes 4}-\frac{2}{15}\sum_{\mathrm{perm}}\delta_{ab}\delta_{cd}\bigotimes_{\mu=a,b,c,d}\mathbf{e}_\mu, \tag{4.33}$$

where we have subtracted the isotropic trace-part for convenience ("perm" denotes the summation over all non-equivalent pairings of the indices of the Kronecker delta functions).

However, these two tensors are not independent. Due the $O(3)$ relations Eq. (4.26), they satisfy

$$\mathbb{B}_1^{D_{4h}}+\mathbb{B}_2^{D_{4h}} = (\mathbf{l}^{\otimes 2}+\mathbf{m}^{\otimes 2})^{\otimes 2} = (\mathbb{1}-\mathbf{n}^{\otimes 2})^{\otimes 2}. \tag{4.34}$$

This in turn means that both $\mathbb{B}_1^{D_{4h}}$ and $\mathbb{B}_2^{D_{4h}}$ have dependence on the axial axis $\mathbf{n}$. Therefore, similarly to the D_{2h} case, it is more convenient to use the linear combination $\mathbb{B}_1^{D_{4h}}-\mathbb{B}_2^{D_{4h}}$ to characterize a D_{4h} order.

In case of C_{6h} symmetry, the biaxial order parameters are rank-6 tensor and defined by the local contractions

$$\sim \mathrm{Tr}\Big[\mathbb{B}_{1,i}^{D_{6h}}\cdot\mathbb{B}_{1,j}^{D_{6h}}+\mathbb{B}_{2,i}^{D_{6h}}\cdot\mathbb{B}_{2,j}^{D_{6h}}+\mathbb{B}_{1,i}^{C_{6h}}\cdot\mathbb{B}_{1,j}^{C_{6h}}+\mathbb{B}_{2,i}^{C_{6h}}\cdot\mathbb{B}_{2,j}^{C_{6h}}\Big], \tag{4.35}$$

up to constant factors and terms depending on the axial axis $\mathbf{n}$, where the explicit form of these tensors are given in Table 4.1. The D_{6h} order parameters appear here since $D_{6h}/C_{6h}\simeq\{\mathbb{1},c_2(\mathbf{l})\}$ is a multiplicative group of order two acting trivially at even powers, leading to redundancy at even orders of the expansion Eq. (4.7). The same phenomenon of course occurs for the C_6 quotients of $\{C_{6v}, D_6, D_{6h}\}$, etc., and the sixth order expansions coincide for the groups with identical order parameters.

Again due to the $O(3)$ relation Eq. (4.26) and Eq. (4.2), these order parameters are not independent. $\mathbb{B}_1^{D_{6h}} + \mathbb{B}_2^{D_{6h}} = (\mathbf{l}^{\otimes 2} + \mathbf{m}^{\otimes 2})^{\otimes 3} = (\mathbb{1} - \mathbf{n}^{\otimes 2})^{\otimes 3}$ depends solely on $\mathbf{n}$, and $\mathbb{B}_1^{C_{6h}} - \mathbb{B}_2^{C_{6h}}$ can be expressed as a function of the pseudovector $\tilde{\mathbf{n}}$. As a consequence, the linear combination $\mathbb{B}_1^{D_{6h}} - \mathbb{B}_2^{D_{6h}}$ and $\mathbb{B}_1^{C_{6h}} + \mathbb{B}_2^{C_{6h}}$ are the appropriate in-plane order parameters for these symmetries.

The above procedure of deriving the biaxial order parameter is valid for all axial nematics with finite n-fold rotational symmetries. Naturally, the rank of the biaxial order parameter tensor increases with n and becomes infinite when $n \to \infty$. This reflects the fact that a biaxial order parameter does not exist for phases with an in-plane $SO(2)$ symmetry, $\{C_\infty, C_{\infty v}, C_{\infty h}, D_\infty, D_{\infty h}\}$.

4.3.3 Polyhedral nematics

Let us finally discuss the order parameters for the polyhedral groups.

Tetrahedral symmetries T, T_d and T_h

The proper tetrahedral group T can be generated by a two-fold rotation $c_2(\mathbf{n})$, as that in Eq. (4.27), and a three-fold rotation acting as a cyclic permutation of $\{\mathbf{l}, \mathbf{m}, \mathbf{n}\}$ given by

$$c_3(\mathbf{l} + \mathbf{m} + \mathbf{n}) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}. \tag{4.36}$$

These result in 12 proper rotations that leave a tetrahedron embedded in a cube with normals $\mathbf{l}, \mathbf{m}, \mathbf{n}$ invariant. After summing over gauge fields $U_{ij} \in T$ in the expansion Eq. (4.7), one finds in the third order the following local contractions,

$$\begin{aligned} &\sim \sigma_i \sigma_j \mathrm{Tr}\Big[\Big(\tilde{\mathbf{l}} \otimes \tilde{\mathbf{m}} \otimes \tilde{\mathbf{n}}\Big)_i \cdot \Big(\sum_{\mathrm{cyc}} \tilde{\mathbf{l}} \otimes \tilde{\mathbf{m}} \otimes \tilde{\mathbf{n}}\Big)_j\Big] \\ &= \frac{1}{3}\mathrm{Tr}\Big[\Big(\sum_{\mathrm{cyc}} \mathbf{l} \otimes \mathbf{m} \otimes \mathbf{n}\Big)_i \cdot \Big(\sum_{\mathrm{cyc}} \mathbf{l} \otimes \mathbf{m} \otimes \mathbf{n}\Big)_j\Big], \end{aligned} \tag{4.37}$$

where $\sum_{\text{cyc}}$ runs over cyclic permutations of $\{\mathbf{l}, \mathbf{m}, \mathbf{n}\}$. Hence we can define the T-invariant local tensor,

$$\mathbb{O}^T = \mathbb{O}_1^T = \sum_{\text{cyc}} \mathbf{l} \otimes \mathbf{m} \otimes \mathbf{n}. \tag{4.38}$$

$\mathbb{O}^T$ in Eq. (4.38) contains only cyclic permutations of the three local axes and carries a chirality, as there are no improper operations in the T group. By interchanging two of these axes corresponding to a reflection, we obtain an equivalent T-invariant tensor but with different handedness,

$$\mathbb{O}_2^T = \sum_{\text{cyc}} \mathbf{m} \otimes \mathbf{l} \otimes \mathbf{n}. \tag{4.39}$$

One realizes that a linear combination of $\mathbb{O}_1^T$ and $\mathbb{O}_2^T$ will give an ordering tensor that is invariant under the symmetry group of a regular tetrahedron, T_d. Indeed, integrating out the gauge fields for the T_d group, where $T_d = T \rtimes \{\mathbb{1}, \sigma_d\}$ and σ_d defined in Eq. (4.27) generating the odd permutation, one will find in the third order of Eq. (4.7)

$$\begin{aligned}
&\sim \sigma_i \sigma_j \operatorname{Tr}\left[\left(\tilde{\mathbf{l}} \otimes \tilde{\mathbf{m}} \otimes \tilde{\mathbf{n}}\right)_i \cdot \Big[\sum_{\text{cyc}} (\tilde{\mathbf{l}} \otimes \tilde{\mathbf{m}} + \tilde{\mathbf{m}} \otimes \tilde{\mathbf{l}}) \otimes \tilde{\mathbf{n}}\Big]_j\right] \\
&= \frac{1}{6} \operatorname{Tr}\left[\Big[\sum_{\text{cyc}} (\mathbf{l} \otimes \mathbf{m} + \mathbf{m} \otimes \mathbf{l}) \otimes \mathbf{n}\Big]_i \cdot \Big[\sum_{\text{cyc}} (\mathbf{l} \otimes \mathbf{m} + \mathbf{m} \otimes \mathbf{l}) \otimes \mathbf{n}\Big]_j\right]
\end{aligned} \tag{4.40}$$

giving precisely the order parameter tensor

$$\mathbb{O}^{T_d} = \sum_{\text{cyc}} (\mathbf{l} \otimes \mathbf{m} + \mathbf{m} \otimes \mathbf{l}) \otimes \mathbf{n} \tag{4.41}$$

as expected.

There is yet another point group belonging to the tetrahedral group family, the group T_h. Interestingly, due to $T_h = T \times \{\mathbb{1}, -\mathbb{1}\}$, all odd orders in the expansion Eq. (4.7) vanish and the first non-trivial terms appear in the fourth order with the contractions,

$$\begin{aligned}
\sim &\operatorname{Tr}\Big[\left(\mathbf{l}^{\otimes 4} + \mathbf{m}^{\otimes 4} + \mathbf{n}^{\otimes 4}\right)_i \cdot \left(\mathbf{l}^{\otimes 4} + \mathbf{m}^{\otimes 4} + \mathbf{n}^{\otimes 4}\right)_j\Big] \\
&+ \operatorname{Tr}\Big[\left(\mathbf{l}^{\otimes 2} \otimes \mathbf{m}^{\otimes 2} + \mathbf{m}^{\otimes 2} \otimes \mathbf{n}^{\otimes 2} + \mathbf{n}^{\otimes 2} \otimes \mathbf{l}^{\otimes 2}\right)_i \\
&\cdot \left(\mathbf{l}^{\otimes 2} \otimes \mathbf{m}^{\otimes 2} + \mathbf{m}^{\otimes 2} \otimes \mathbf{n}^{\otimes 2} + \mathbf{n}^{\otimes 2} \otimes \mathbf{l}^{\otimes 2}\right)_j\Big].
\end{aligned} \tag{4.42}$$

The second term in the above expression gives the T_h invariant order parameter tensor

$$
\begin{aligned}
\mathbb{O}^{T_h} &= \mathbb{O}_1^{T_h} \\
&= \mathbf{l}^{\otimes 2} \otimes \mathbf{m}^{\otimes 2} + \mathbf{m}^{\otimes 2} \otimes \mathbf{n}^{\otimes 2} + \mathbf{n}^{\otimes 2} \otimes \mathbf{l}^{\otimes 2} - \frac{2}{5}\delta_{ab}\delta_{cd} \bigotimes_{\mu=a,b,c,d} \mathbf{e}_\mu \\
&\quad + \frac{1}{10}\Big(\delta_{ac}\delta_{bd} \bigotimes_{\mu=a,c,b,d} \mathbf{e}_\mu + \delta_{ad}\delta_{bc} \bigotimes_{\mu=a,d,b,c} \mathbf{e}_\mu\Big),
\end{aligned}
\tag{4.43}
$$

where we have subtracted the trace. The first term in Eq. (4.42) actually coincides with the O_h ordering tensor $\mathbb{O}^{O_h}$. This is because $O_h/T_h \simeq \{\mathbb{1}, -\sigma_d\}$ is a group of order two that leads to some redundant information at even orders in the expansion. $\mathbb{O}^{T_h}$ in Eq. (4.43) is not invariant under interchanging $\mathbf{l}$ and $\mathbf{m}$, which corresponds to the four fold rotation in O_h. Therefore, we can define another T_h-invariant tensor,

$$
\begin{aligned}
\mathbb{O}_2^{T_h} &= \mathbf{m}^{\otimes 2} \otimes \mathbf{l}^{\otimes 2} + \mathbf{n}^{\otimes 2} \otimes \mathbf{m}^{\otimes 2} + \mathbf{l}^{\otimes 2} \otimes \mathbf{n}^{\otimes 2} - \frac{2}{5}\delta_{ab}\delta_{cd} \bigotimes_{\mu=a,b,c,d} \mathbf{e}_\mu \\
&\quad + \frac{1}{10}\Big(\delta_{ac}\delta_{bd} \bigotimes_{\mu=a,c,b,d} \mathbf{e}_\mu + \delta_{ad}\delta_{bc} \bigotimes_{\mu=a,d,b,c} \mathbf{e}_\mu\Big).
\end{aligned}
\tag{4.44}
$$

Due to the $O(3)$ constraints, however, this and the two terms in Eq. (4.42) are not independent,

$$
\begin{aligned}
&\mathbb{O}^{O_h} + \mathbb{O}_1^{T_h} + \mathbb{O}_2^{T_h} \\
&= (\mathbf{l}\otimes\mathbf{l} + \mathbf{m}\otimes\mathbf{m} + \mathbf{n}\otimes\mathbf{n})^{\otimes 2} + const. \\
&= \mathbb{1}\otimes\mathbb{1} + const..
\end{aligned}
\tag{4.45}
$$

Therefore, both $\mathbb{O}_1^{T_h}$ and $\mathbb{O}_2^{T_h}$ suffice to describe the T_h orientational order.

Cubic symmetries O and O_h

The O group consists of all 24 proper rotations leaving a cube invariant, and O_h in addition contains inversions, $O_h = O \times \{\mathbb{1}, -\mathbb{1}\}$, and thus in total has 48 elements. A set of generators for O_h is given by $\{c_4(\mathbf{n}), c_3(\mathbf{l}+\mathbf{m}+\mathbf{n}), c_2(\mathbf{m}+\mathbf{n}), -\mathbb{1}\}$, where $c_3(\mathbf{l}+\mathbf{m}+\mathbf{n})$ is defined in Eq. (4.36), and $c_4(\mathbf{n})$ and $c_2(\mathbf{m}+\mathbf{n})$ are given as

$$
c_4(\mathbf{n}) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \; c_2(\mathbf{m}+\mathbf{n}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.
\tag{4.46}
$$

Non-zero terms for O_h appear likewise in fourth order of the expansion Eq. (4.7) and now one will obviously find the same contraction as the first term in Eq. (4.42) up to some a constant factor, hence one can define the O_h order parameter tensor as

$$\mathbb{O}^{O_h} = \mathbf{l}^{\otimes 4} + \mathbf{m}^{\otimes 4} + \mathbf{n}^{\otimes 4} - \frac{1}{5} \sum_{\text{perm}} \delta_{ab}\delta_{cd} \bigotimes_{\mu=a,b,c,d} \mathbf{e}_\mu. \tag{4.47}$$

For the proper subgroup O, we have an additional non-trivial third order in the expansion, which is simply $\sim \sigma_i \sigma_j$ giving the chiral order parameter.

Icosahedral symmetries I and I_h

The icosahedral group I consists of all 60 proper rotations that leave a icosahedron invariant and $I_h = I \times \{\mathbb{1}, -\mathbb{1}\}$ contains additionally 60 improper rotations. An icosahedron centered at $(0, 0, 0)$ can be defined by its 12 vertexes at [132]

$$(\pm\frac{1}{2},\ 0,\ \pm\frac{\tau}{2}), (\pm\frac{\tau}{2},\ \pm\frac{1}{2},\ 0), (0,\ \pm\frac{\tau}{2},\ \pm\frac{1}{2}), \tag{4.48}$$

where $\tau = (\sqrt{5}+1)/2$ is the golden ratio. It is invariant under a five fold rotations about its six diagonals. The axis $\mathbf{l} + \tau\mathbf{n}$ is the diagonal passing trough vertices $(-\frac{1}{2}, 0, -\frac{\tau}{2})$ and $(\frac{1}{2}, 0, \frac{\tau}{2})$. A set of generators of I_h is given by $\{c_5(\mathbf{l}+\tau\mathbf{n}), c_3(\mathbf{l}+\mathbf{m}+\mathbf{n}), c_2(\mathbf{n}), -\mathbb{1}\}$, where $c_3(\mathbf{l}+\mathbf{m}+\mathbf{n})$ and $c_2(\mathbf{n})$ are defined in Eq. (4.36) and Eq. (4.27), respectively, $c_5(\mathbf{l}+\tau\mathbf{n})$ is given by

$$c_5(\mathbf{l}+\tau\mathbf{n}) = \begin{pmatrix} 1/2 & -\tau/2 & 1/(2\tau) \\ \tau/2 & 1/(2\tau) & -1/2 \\ 1/(2\tau) & 1/2 & \tau/2 \end{pmatrix}. \tag{4.49}$$

The minimal non-trivial I_h invariant tensor appears in the sixth order in the expansion Eq. (4.7), leading to a rank-6 tensor,

$$\begin{aligned} \mathbb{O}^{I_h} = \sum_{\text{cyc}} \Big[\mathbf{l}^{\otimes 6} + \sum_{\{+,-\}} \Big(\frac{1}{2}\mathbf{l} \pm \frac{\tau}{2}\mathbf{m} \pm \frac{1}{2\tau}\mathbf{n} \Big)^{\otimes 6} \Big] \\ - \frac{1}{7} \sum_{\text{perm}} \delta_{ab}\delta_{cd}\delta_{ef} \bigotimes_{\substack{\mu=a,b,c,\\ d,e,f}} \mathbf{e}_\mu. \end{aligned} \tag{4.50}$$

Moreover, similar to the O-nematic case, an I-invariant order parameter consists of an orientational part and a chiral part and is accordingly defined as $\mathbb{O}^I = \{\mathbb{O}^{I_h}, \sigma\}$.

4.4 Concluding remarks

The rotational symmetries of three dimensional isotropic space $O(3)$ can in principle break to any non-trivial point group. According to the Landau-de Gennes paradigm, each symmetry is accompanied by a order parameter and associated phase transitions. These order parameters are high-rank tensors and quite involved in general. In virtue of the gauge theory introduced in previous chapter, we have developed a systematic way of classifying these order parameter tensors and have presented the explicit form of these order parameters for an extensive selection of the physically most relevant symmetries. Although we arrived at these results utilizing a particular gauge theoretical lattice model, the results are of course independent of the gauge theoretical machinery. With these order parameters it is in principle possible to study the nematic phases via Landau-de Gennes theories by considering all symmetry allowed couplings of the order parameters, for example using the approach outlined in Ref. [91]. Given the universality of the applications of the orientational tensor order parameters our work is of general interest for many different fields; in particular we anticipate that our results can provide for a road map for the search of new nematic phases of matter.