Octupolar tensors for liquid crystals

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Abstract
A third-rank three-dimensional symmetric traceless tensor, called the octupolar tensor, has been introduced to study tetrahedric nematic phases in liquid crystals. The octupolar potential, a scalar-valued function generated on the unit sphere by that tensor, should ideally have four maxima (on the vertices of a tetrahedron), but it was recently found to possess an equally generic variant with three maxima instead of four. It was also shown that the irreducible admissible region for the octupolar tensor in a three-dimensional parameter space is bounded by a dome-shaped surface, beneath which is a separatrix surface connecting the two generic octupolar states. The latter surface, which was obtained through numerical continuation, may be physically interpreted as marking a possible intra-octupolar transition. In this paper, by using the resultant theory of algebraic geometry and the E-characteristic polynomial of spectral theory of tensors, we give a closed-form, algebraic expression for both the dome-shaped surface and the separatrix surface. This turns the envisaged intra-octupolar transition into a quantitative, possibly observable prediction.

Keywords: liquid crystals, octupolar order tensors, resultants

(Some figures may appear in colour only in the online journal)
1. Introduction

Liquid crystals are well-known for their applications in flat panel electronic displays. But beyond that, various optical and electronic devices, such as laser printers, light-emitting diodes, field-effect transistors, and holographic data storage, were invented with the development of bent-core (banana-shaped) liquid crystals [8, 9]. These liquid crystal phases are characterized by a third-rank, three-dimensional, symmetric traceless tensor $A$ first introduced in [6] to characterize condensed phases exhibited by bent-core molecules [11, 15]. We shall call $A$ the octupolar tensor.

Based on such a tensor, an orientationally ordered octupolar (tetrahedratic) phase has been both predicted theoretically [2, 13] and confirmed experimentally [28]. Octupolar order parameters of liquid crystals have recently been widely studied [1, 7]. Generalized liquid crystal phases were also considered in [12, 16], which feature octupolar order tensors among many others.

Broadly, there are two types of octupolar order: one arising from complex molecular architectures, and the other arising from a more refined description of the orientational distribution of simple, rod-like molecules. In both cases, the algebraic properties of $A$ are the same. So the same tensor would represent the ordering of tetrahedratic nematic molecules as well as the cubic term in Buckingham’s formula [3, 26] for the expansion in Cartesian tensors of the orientational probability density function for uniaxial nematics.

Virga [27] and Gaeta and Virga [7], in their studies of octupolar tensors in two and three space dimensions, also introduced the octupolar potential, a scalar-valued function on the unit sphere obtained from the octupolar tensor. In particular, Gaeta and Virga [7] showed that the irreducible admissible region for the octupolar potential is bounded by a surface in a three-dimensional parameter space which has the form of a dome and, more importantly, that there are indeed two generic octupolar states, divided by a separatrix surface in parameter space. Physically, the latter surface was interpreted as representing a possible intra-octupolar transition.

In this paper, by using the resultant theory of algebraic geometry and the E-characteristic polynomial of the spectral theory of tensors, we give a closed-form, algebraic expression for both the dome and the separatrix. This turns the intra-octupolar transition envisioned in [7] into a quantitative, possibly observable prediction.

In section 2, we recall from [13] how to define octupolar order parameters in the case of complex molecular architectures. In section 3, we collect a number of algebraic preliminaries to make our development self-contained. In particular, we reduce the independent elements of the octupolar tensor $A$ from seven to three by assuming that the North pole $(0, 0, 1)^\top$ is a maximum point of the octupolar potential on the unit sphere. In section 4, we present an algebraic geometry method to compute the resultant of multi-polynomial systems [5]. As an example, we derive the determinant of $A$, which is the resultant $\text{Res}(Ax^2)$. In section 5, by assuming that the North pole $(0, 0, 1)^\top$ is the global maximum point of the octupolar potential on the unit sphere, the admissible region is further reduced. The boundary of such a reduced admissible region was referred to as the dome in [7]. By resorting to the algebraic geometry notion of E-characteristic polynomial $\phi_A(\lambda)$ of $A$, we arrive at the explicit expression for both the dome and the separatrix, which in [7] were only determined by numerical continuation. Finally, a quick recapitulation of our results is recorded in section 6. A technical appendix then closes the paper.

2. Octupolar order parameters

Describing the wealth of phases made possible by soft matter physics requires primarily identifying the appropriate order parameters capable of translating into a mesoscopic language the descriptors of the microscopic, molecular structure. Many accounts are given in the literature on this central issue; the reader is in particular referred to [18] for its explicit pedagogical intent.
Nematic liquid crystals are perhaps the simplest and most classical examples of phases requiring a non-scalar order parameter. Typically a nematic molecule is with good approximation linear and enjoy (on average) the head-tail symmetry, which is more properly represented as the invariance under a reflection. Therefore, if $\mathbf{a}$ is a unit vector along the symmetry axis, the natural molecular descriptor is the second-rank tensor $\mathbf{a} \otimes \mathbf{a}$, where a superimposed $\cdot \cdot \cdot$ denotes the traceless, symmetric component of the tensor it surmounts. An organized nematic phase will then be described by the quadrupolar order tensor

$$\mathbf{Q} := \langle \mathbf{a} \otimes \mathbf{a} \rangle,$$

where the brackets $\langle \cdot \cdot \cdot \rangle$ denote an ensemble average.

All this is very well-known and can be found in several textbooks (among the many, we refer the reader in particular to chapter 1 of [24] for its treatment of the mean-field side of the story). We only heed that $\mathbf{Q}$, despite being the average of a uniaxial tensor (with two equal eigenvalues), may fail to be so (because the eigenvalues of a tensor do not depend linearly on the tensor). When the molecular architecture is more articulated, the picture becomes correspondingly more complicated. Second-rank tensors may no longer suffice to describe the molecular structure, even when this is assumed to be rigid (which is by itself a strong assumption). To explain this, we shall consider a simple molecular model, which is particularly germane to the algebraic topic at hand.

Following a paper that has already become a classic in this field [13], we consider a molecule consisting of three atoms not lying on a line. They are arranged in a V-shaped fashion, as shown in figure 1, with identical terminal atoms. For simplicity, only steric interactions are considered between such molecules, so that only geometric parameters and masses may count. Letting $a$ be the length of each arm of the ‘V’ and $\alpha$ the angle between the arms, we denote by $m$ the mass of the atoms at the ends and by $M$ the mass of the atom at the vertex. We further call $\mathbf{a}_2$ a unit vector along the direction joining the ends and $\mathbf{a}_1$ a unit vector along the symmetry axis through the vertex (see figure 1). The point symmetry group of such V-shaped molecules is $C_2v$: it consists of two reflections and one $\pi$-rotation.

Though specifically applied to molecules enjoying this symmetry, the theory presented in [13] has in principle a much broader scope. It is predicated on the assumption that only tensors extracted from the mass distribution in a constituent molecule are relevant to molecular interactions. In general, for a molecule with $N$ atoms with masses $m_\mu$, $\mu = 1, \ldots, N$, located at points designated by the position vectors $\mathbf{r}_\mu$ relative to the molecule’s centre of mass, the bare structural tensors $\mathbf{A}(m)$ are defined by

$$\mathbf{A}(m) := \sum_{\mu=1}^{N} m_\mu \mathbf{r}_\mu^\otimes m,$$

where $\mathbf{r}_\mu^\otimes m$ is the $m$th-rank tensor

$$\mathbf{r}_\mu^\otimes m := \underbrace{\mathbf{r}_\mu \otimes \cdots \otimes \mathbf{r}_\mu}_{m \text{ times}}.$$

It follows immediately from (1) that $\mathbf{A}(1) = 0$, and so if any vector is to be listed among the order tensors of this system, it must come from the trace of some higher-rank tensor. The first candidate is of course $\mathbf{A}(3)$, and so we may define formally the vector

$$\mathbf{C}(1) := \mathbf{I} \cdot \mathbf{A}(3),$$
where $\mathbf{I}$ is the second-rank identity and $\cdot$ stands for contraction, so that the components of $\mathbf{C}^{(1)}$ in a generic orthonormal Cartesian frame $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ are given by

$$C_i^{(1)} = \sum_{j=1}^{3} A_{ij}^{(3)}.$$

Further information on the molecular mass distribution is contained in the second- and third-rank tensors defined by

$$\mathbf{C}^{(2)} := \overrightarrow{A}^{(2)} \quad \text{and} \quad \mathbf{C}^{(3)} := \overrightarrow{A}^{(3)}.$$

By exploiting the specific $C_{2v}$ symmetry embodied by the V-shaped molecule depicted in Figure 1, one readily shows that in this case

$$\mathbf{C}^{(1)} = c_{11} \mathbf{a}_1,$$

\begin{align*}
\mathbf{C}^{(2)} &= c_{21} \mathbf{a}_1 \otimes \mathbf{a}_1 + c_{22} \mathbf{a}_2 \otimes \mathbf{a}_2, \\
\mathbf{C}^{(3)} &= c_{31} \mathbf{a}_1 \otimes \mathbf{a}_1 \otimes \mathbf{a}_1 + c_{32} \mathbf{a}_2 \otimes \mathbf{a}_2 \otimes \mathbf{a}_1,
\end{align*}

where the coefficients $c_{ij}$ are explicitly related to the molecular parameters $m$, $M$, $a$, and $\alpha$ [13]. This shows the dual role played by third-rank tensors in the description of more complex molecular architectures: they introduce two independent measures of shape polarity, $\mathbf{C}^{(1)}$ and $\mathbf{C}^{(3)}$. 

**Figure 1.** Cartoon representing a three-atomic, V-shaped molecule enjoying the $C_{2v}$ symmetry. The length of each arm of the ‘V’ is $a$, while the angle between the arms is $\alpha$. The double arrow in the unit vector $\mathbf{a}_2$ suggests that the two ends of the molecule are symmetric, and so $\mathbf{a}_2$ and $-\mathbf{a}_2$ are equivalent, whereas the unit vector $\mathbf{a}_1$ along the symmetry axis cannot be reversed without affecting the molecule’s structure. The mass of both terminal atoms is $m$, whereas the mass of the atom at the vertex is $M$. 

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In a purely entropic theory, such as the one first formulated by Onsager [17], steric interactions are embodied by the excluded volume between two molecules, which becomes an effective pair-potential. The role of shape tensors such as \( C^{(2)} \) and \( C^{(3)} \) in representing the excluded volume of \( C_{\infty v} \) (conical) molecules has already been illuminated in [19]. Although, to our knowledge, a similar study is not yet available for \( C_{2v} \) molecules, we expect the excluded volume of the latter to be expressible in terms of both independent tensorial components featuring in \( C^{(2)} \) and \( C^{(3)} \) as represented in (2b) and (2c), respectively. Thus, the quadrupolar order tensors now defined as

\[
Q_i := \langle a_i \otimes a_i \rangle, \quad i = 1, 2,
\]

are supplemented by the octupolar companions

\[
A_1 := \langle a_2 \otimes a_2 \otimes a_1 \rangle \quad \text{and} \quad A_2 := \langle a_1 \otimes a_1 \otimes a_1 \rangle.
\]

Both types of tensors are fully symmetric and traceless. We shall generically refer to them as \( Q \) and \( A \), as they have just the same algebraic properties.

In a given frame \( \{e_1, e_2, e_3\} \), \( Q \) can be represented by 5 independent parameters, while \( A \) can be represented by 7 independent parameters. Properly speaking, however, these are not scalar order parameters, as they are not invariant under frame rotations. If it is well known that the scalar order parameter associated with \( Q \) are its eigenvalues, it is not equally clear what they should be for \( A \), as different notions of (nonlinear) eigenvalues have been introduced for higher-rank tensors. As shown in more details below, in our approach, which is reprised from [7], the scalars that best describe \( A \) are the critical values of a potential \( \Phi \) on the unit sphere \( S^2 \) associated with \( A \), which we shall call the octupolar potential (see equation (5) below).

In [7], special attention was given to the maxima of \( \Phi \) (which symmetry demands to be opposite to the minima). It was shown that in general \( \Phi \) may possess either 4 or 3 maxima, both cases being generic and corresponding to two distinguishable subphases. Peculiar illustrations of these cases are shown in figure 2, where polar plots of \( \Phi \) are illuminated which enjoy the tetrahedral symmetry \( T_d \) and the dihedral symmetry \( D_{3h} \), respectively.

In particular, the \( T_d \) symmetry is at the basis of both theoretical [2, 6, 25] and simulation [23] studies of the tetrahedratic phases explored so far. It was shown in [7] that this is by far too specific a phase among those that can be described by an octupolar order tensor: there are two generic classes of such phases; they can intuitively be visualized by distorting the potential plots shown in figure 1, making their maxima unequal, while preserving their number. It is the objective of this paper to describe exactly the transition between these two types of octupolar order.

### 3. Algebraic preliminaries

We collect in this section a number of preliminary results to make the reader acquainted with the theory of higher-rank tensors.

#### 3.1. Octupolar tensors

The octupolar tensor \( A \) for liquid crystals is a symmetric, traceless tensor in three space dimensions [13, 26]. To set the scene for our formal development, we first give the general definition of a traceless tensor.
Definition 3.1. Let $T = [t_{i_1 i_2 ... i_m}] \in \mathbb{R}^{[m,n]}$ be a symmetric tensor. If
$$
\sum_{i=1}^{n} t_{i_1 i_2 ... i_m} = 0
$$
for all $i_3, ..., i_m = 1, 2, ..., n$, then $T$ is called a symmetric traceless tensor.

The following theorem, whose proof will be omitted, shows that the traceless property of a symmetric tensor is invariant under orthogonal transformations [7].

Theorem 3.2. Let $T = [t_{i_1 i_2 ... i_m}] \in \mathbb{R}^{[m,n]}$ be a symmetric traceless tensor and $Q = [q_{ij}] \in \mathbb{R}^{n \times n}$ be an orthogonal matrix. We denote by $TQ^m \in \mathbb{R}^{[m,n]}$ the symmetric tensor whose elements are
$$
[TQ^m]_{i_1 i_2 ... i_m} = \sum_{j_1=1}^{n} \sum_{j_2=1}^{n} ... \sum_{j_m=1}^{n} t_{j_1 j_2 ... j_m} q_{i_1 j_1} q_{i_2 j_2} ... q_{i_m j_m}.
$$

Then, $TQ^m$ is also a symmetric traceless tensor.

By exploiting the rotational invariance of traceless tensors, we now represent the octupolar tensor

$$
A = \begin{bmatrix}
    a_{111} & a_{112} & a_{113} \\
    a_{121} & a_{122} & a_{123} \\
    a_{131} & a_{132} & a_{133}
\end{bmatrix}
\begin{bmatrix}
    a_{111} & a_{112} & a_{113} \\
    a_{121} & a_{122} & a_{123} \\
    a_{131} & a_{132} & a_{133}
\end{bmatrix}
\begin{bmatrix}
    a_{111} & a_{112} & a_{113} \\
    a_{121} & a_{122} & a_{123} \\
    a_{131} & a_{132} & a_{133}
\end{bmatrix}
\begin{bmatrix}
    a_{111} & a_{112} & a_{113} \\
    a_{121} & a_{122} & a_{123} \\
    a_{131} & a_{132} & a_{133}
\end{bmatrix}
\in \mathbb{R}^{[3,3]}
$$

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    a_{121} & a_{122} & a_{123} \\
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\end{bmatrix}
\begin{bmatrix}
    a_{111} & a_{112} & a_{113} \\
    a_{121} & a_{122} & a_{123} \\
    a_{131} & a_{132} & a_{133}
\end{bmatrix}
\in \mathbb{R}^{[3,3]}
$$

by choosing a proper Cartesian coordinate system. The traceless property of $A$ means that

$$
\begin{cases}
    a_{111} + a_{122} + a_{133} = 0, \\
    a_{112} + a_{222} + a_{233} = 0, \\
    a_{113} + a_{223} + a_{333} = 0.
\end{cases}
$$

Hence, there are seven independent elements in $A$. Let

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.png}
\caption{Polar plots on the unit sphere $S^2$ of the octupolar potential, defined formally in (5). (a) $\Phi$ has four maxima and enjoys the $T_d$ symmetry. (b) $\Phi$ has three maxima and enjoys the $D_3h$ symmetry.}
\end{figure}
\[ a_0 = a_{123}, \ a_1 = a_{111}, \ a_2 = a_{222}, \ a_3 = a_{333}, \ \beta_1 = a_{122}, \ \beta_2 = a_{233}, \ \beta_3 = a_{113}. \]

Using the traceless property (4), we convert (3) into

\[
A = \begin{bmatrix}
  \alpha_0 & -\alpha_2 & -\beta_1 & -\alpha_2 & -\beta_1 & \alpha_0 & \beta_1 & \alpha_0 & -\alpha_1 - \beta_1 \\
  -\alpha_2 & \beta_1 & \alpha_0 & -\alpha_2 & \beta_1 & \alpha_0 & \beta_1 & \alpha_0 & -\alpha_1 - \beta_1 \\
  \beta_3 & \alpha_0 & -\alpha_1 - \beta_1 & \beta_3 & \alpha_0 & -\alpha_1 - \beta_1 & \beta_3 & \alpha_0 & -\alpha_1 - \beta_1 \\
  \end{bmatrix}.
\]

The associated octupolar potential as defined in [7] is

\[
\Phi(x) := A x^3
= \alpha_1 x_1^3 + \alpha_2 x_2^3 + \alpha_3 x_3^3 + 6\alpha_0 x_1 x_2 x_3 + 3\beta_1 x_1 x_2^2 + 3\beta_2 x_2 x_3^2 + 3\beta_3 x_3 x_1^2
- 3(\alpha_1 + \beta_1) x_1 x_2^2 - 3(\alpha_2 + \beta_2) x_2 x_3^2 - 3(\alpha_3 + \beta_3) x_3 x_1^2.
\]

(5)

On the unit sphere \( S^2 := \{ x = (x_1, x_2, x_3)^T : x_1^2 + x_2^2 + x_3^2 = 1 \} \), the polynomial \( \Phi(x) \) has at least one maximum point. Without loss of generality, we assume such a maximum point to be the North pole \( (0, 0, 1)^T \) and that

\[ \alpha_3 = \Phi(0, 0, 1) \geq 0. \]

By this assumption, the North pole \( (0, 0, 1)^T \) is a critical point of \( \Phi \) and must satisfy the following system of equations for a suitable number \( \lambda \):

\[
\begin{aligned}
\alpha_1 x_1^3 + 2\alpha_0 x_2 x_3 + \beta_1 x_2^3 + 2\beta_2 x_1 x_3 - (\alpha_1 + \beta_1) x_1 x_2^2 - 2(\alpha_2 + \beta_2) x_1 x_2 x_3 &= \lambda x_1, \\
\alpha_2 x_2^3 + 2\alpha_0 x_1 x_3 + 2\beta_1 x_1 x_2 + \beta_2 x_1^3 - (\alpha_2 + \beta_2) x_1^2 x_2 - 2(\alpha_3 + \beta_3) x_1 x_2 x_3 &= \lambda x_2, \\
\alpha_3 x_3^3 + 2\alpha_0 x_1 x_2 + 2\beta_2 x_2 x_3 + \beta_3 x_2^3 - 2(\alpha_1 + \beta_1) x_1 x_3 - (\alpha_3 + \beta_3) x_2^2 &= \lambda x_3, \\
x_1^2 + x_2^2 + x_3^2 &= 1.
\end{aligned}
\]

(6)

Hence, requiring \((0, 0, 1)^T\) to be a solution, we obtain

\[ \alpha_1 + \beta_1 = 0 \quad \text{and} \quad \beta_2 = 0. \]

Moreover, because \( \Phi(-x_1, 0, 0) = -\Phi(x_1, 0, 0) \), we can rotate the Cartesian coordinate system so that \( \Phi(1, 0, 0) = 0 \) and we get

\[ \alpha_1 = 0. \]

Now, the octupolar tensor in (3) reduces to

\[
A = \begin{bmatrix}
  0 & -\alpha_2 & -\beta_3 & -\alpha_2 & 0 & \alpha_0 & \beta_3 & \alpha_0 & 0 \\
  -\alpha_2 & 0 & \alpha_0 & -\alpha_2 & 0 & \alpha_0 & -\alpha_3 - \beta_3 & 0 & 0 \\
  \beta_3 & \alpha_0 & 0 & 0 & \alpha_0 & -\alpha_3 - \beta_3 & 0 & 0 & \alpha_3 \\
  \end{bmatrix},
\]

which features four independent elements, namely, \( \alpha_0, \alpha_2, \alpha_3, \) and \( \beta_3 \). Correspondingly, the octupolar potential (5) is

\[
\Phi(x; \alpha_0, \alpha_2, \alpha_3, \beta_3) = \alpha_2 x_2^3 + \alpha_3 x_3^3 + 6\alpha_0 x_1 x_2 x_3 + 3\beta_3 x_1 x_2^2 x_3 - 3\alpha_2 x_1^2 x_2 - 3(\alpha_3 + \beta_3) x_2^2 x_3
\]

for all \( x \in S^2 \). Without loss of generality, we can assume

\[ \alpha_2 \geq 0 \]

as a consequence of the following proposition.
Proposition 3.3. For the octupolar potential (5), we have

\[ \Phi(x_1, x_2, x_3; \alpha_0, \alpha_2, \alpha_3, \beta_3) = \Phi(x_1, -x_2, x_3; -\alpha_0, -\alpha_2, \alpha_3, \beta_3). \]

Next, we enforce the condition that the North pole \((0, 0, 1)^T\) is a maximum point of the octupolar potential with value \(\alpha_3\). The following theorem is proven in [7].

Theorem 3.4. Suppose that the North pole \((0, 0, 1)^T\) is a local maximum point of the octupolar potential \(\Phi(x)\) on \(S^2\). Then, we have that

\[ 3\alpha_3^2 - 4\alpha_3\beta_3 - 4\beta_3^2 - 4\alpha_0^2 \geq 0. \]  

(7)

We first consider the case that \(\alpha_3 = 0\). From theorem 3.4, we know that \(\alpha_0 = \beta_3 = 0\). If \(\alpha_2 > 0\), then \(\Phi(0, 1, 0) = \alpha_2 > \alpha_3 = \Phi(0, 0, 1)\). This contradicts that \((0, 0, 1)^T\) is a maximum point. Hence \(\alpha_2 = 0\) and the octupolar tensor \(A\) is the trivial zero tensor.

In the remainder of this paper, we shall consider the case that \(\alpha_3\) is positive. Without loss of generality, by proposition 3.3 and theorem 3.4, we can choose \(\alpha_3 = 1\), \(\alpha_2 \geq 0\), and \(\alpha_0^2 + (\beta_3 + \frac{1}{2})^2 \leq 1\).

(8)

Then, the octupolar tensor

\[ A(\alpha_0, \beta_3, \alpha_2) = \begin{bmatrix} 0 & -\alpha_2 & \beta_3 & -\alpha_2 & 0 & \alpha_0 & \beta_3 & \alpha_0 & 0 \\ -\alpha_2 & 0 & \alpha_0 & 0 & \alpha_2 & -1 - \beta_3 & \alpha_2 & -1 - \beta_3 & 0 \\ \beta_3 & \alpha_0 & 0 & \alpha_0 & -1 - \beta_3 & 0 & 0 & 0 & 1 \end{bmatrix}, \]

(9)

has only three independent elements and the associated octupolar potential is given by

\[ \Phi(x) = \alpha_2 x_2^2 + x_3^3 + 6\alpha_0 x_1 x_2 x_3 + 3\beta_3 x_2^2 x_3 - 3\alpha_2 x_1^2 x_2 - 3(1 + \beta_3) x_2^2 x_3 \]

(10)

for all \(x \in S^2\).

3.2. Spectral tensor theory

Our analysis of the critical points of \(\Phi\) presented in the following sections relies on a number of general notions of algebraic geometry, which we now recall to make our presentation self-contained.

Let \(m \geq 3\) and \(n \geq 2\) be integers. We denote as \(\mathbb{R}^{[m,n]}\) the real-valued space of \(m\)th-rank, \(n\)-dimensional, symmetric tensors. Given \(T = [t_{ij\cdots i_n}] \in \mathbb{R}^{[m,n]}\) and \(x \in \mathbb{R}^n\), we define a scalar

\[ Tx^m := \sum_{i_1=1}^{n} \sum_{i_2=1}^{n} \cdots \sum_{i_m=1}^{n} t_{i_1i_2\cdots i_m} x_{i_1} x_{i_2} \cdots x_{i_m} \]

and a vector \(Tx^{m-1} \in \mathbb{R}^n\) whose \(j\)th element is

\[ [Tx^{m-1}]_j = \sum_{i_2=1}^{n} \cdots \sum_{i_m=1}^{n} t_{j i_2\cdots i_m} x_{i_2} \cdots x_{i_m}. \]
In [20] (see also [22]), Qi gave the following definition of E-/Z-eigenvalues for symmetric tensors.

**Definition 3.5.** Let $T \in \mathbb{R}^{[m,n]}$. If there exist a number $\lambda \in \mathbb{C}$ and a vector $x \in \mathbb{C}^n$ such that
\[
\begin{cases}
T x^{m-1} = \lambda x, \\
x^\top x = 1,
\end{cases}
\]  
we call $\lambda$ an E-eigenvalue of $T$ and $x$ an E-eigenvector of $T$ associated with $\lambda$.

Furthermore, if there exists a real $x$ satisfying (11), then $\lambda$ is also real. In this case, $\lambda$ is called a Z-eigenvalue of $T$ and $x$ is its associated Z-eigenvector.

It follows from the system (6) that the North pole $(0, 0, 1)^\top$ is a Z-eigenvector of the octupolar tensor $A$ with associated Z-eigenvalue equal to 1.

Let $A \in \mathbb{R}^{n \times n}$. It is well-known that the linear system $Ax = 0$ has non-zero solutions if and only if the determinant $\det(A)$ vanishes. To generalize this result to a multi-polynomial system $F(x) = 0$, we make use of the resultant theory from algebraic geometry [5].

Let $F_1(x), F_2(x), \ldots, F_n(x)$ be homogeneous polynomials of positive degree $d_1, d_2, \ldots, d_n$, respectively. For convenience, we denote $F(x) := (F_1(x), F_2(x), \ldots, F_n(x))^\top$. The resultant of $F(x)$ is an irreducible polynomial in the coefficients of $F_i(x)$’s, which vanishes if and only if the system $F(x) = 0$ has non-zero solutions; if $F_i(x) = x^{d_i}$ for $i = 1, \ldots, n$, the value of the resultant of $F(x)$ is 1. We denote as $\text{Res}(F(x))$ the resultant of $F(x)$ in the remainder of this paper.

**Definition 3.6.** Let $T \in \mathbb{R}^{[m,n]}$. The determinant of $T$ is the resultant $\text{Res}(T x^{m-1})$.

The E-characteristic polynomial $\phi_T(x)$ of $T$ is the resultant of the following system:
\[
\begin{cases}
T x^{m-1} - \lambda x^{m-2} = 0, \\
x^2 - x^\top x = 0.
\end{cases}
\]

More details for the determinant and the E-characteristic polynomial of a symmetric tensor can be found in [22].

If there exists a non-zero vector $x \in \mathbb{C}^n$ such that $T x^{m-1} = 0$ and $x^\top x = 0$, we say that the tensor $T$ is irregular. Otherwise, we say that $T$ is a regular tensor.

**Theorem 3.7.** Let $T \in \mathbb{R}^{[m,n]}$. Then all E-eigenvalues of $T$ are roots of the E-characteristic polynomial $\phi_T(\lambda) = 0$. If $T$ is regular, then $\lambda$ is an E-eigenvalue of $T$ if and only if $\phi_T(\lambda) = 0$.

Qi [20] showed that E-eigenvalues of a symmetric tensor are invariant under orthonormal coordinate changes. E-eigenvalues and E-eigenvectors were further studied in [4, 14, 21] and Furthermore, the coefficients of the E-characteristic polynomial of a tensor were shown to be orthonormal invariants of that tensor [10].

### 4. Algebraic geometry methods

Here we compute explicitly the determinant and the E-characteristic polynomial of the octupolar tensor (9) by using the method of resultants explained in chapter 3, section 4 of [5].
For the determinant of the octupolar tensor $A(\alpha_0, \beta_3, \alpha_2)$, we first calculate
\[
A^2 = \begin{pmatrix}
-2\alpha_0 x_1 x_2 + 2\beta_3 x_1 x_3 + 2\alpha_0 x_2 x_3 \\
-\alpha_2 x_1^2 + \alpha_2 x_2^2 + 2\alpha_0 x_1 x_3 - 2(1 + \beta_3)x_2 x_3 \\
\beta_3 x_1^3 - (1 + \beta_3)x_2^3 + x_3^2 + 2\alpha_0 x_1 x_2
\end{pmatrix} =: \begin{pmatrix}
F_3(x_1, x_2, x_3) \\
F_1(x_1, x_2, x_3) \\
F_2(x_1, x_2, x_3)
\end{pmatrix}.
\]

Clearly, the degree of each of the $F_i$ is $d_i = 2$. Second, we set
\[
d = \sum_{i=1}^{3}(d_i - 1) + 1 = 4
\]
and divide monomials $x^\mu := x_1^{\nu_1} x_2^{\nu_2} x_3^{\nu_3}$ of total degree $|\mu| := \nu_1 + \nu_2 + \nu_3 = d$ into three sets:
$S_1 = \{ x^\mu : |\mu| = d, x_1^3 \text{ divides } x^\mu \} = \{ x_1^4, x_1^3 x_2, x_1^3 x_3, x_1 x_2^2 x_3, x_1^2 x_2 x_3, x_1^2 x_3^2 \},$
$S_2 = \{ x^\mu : |\mu| = d, x_1^3 \text{ does not divides } x^\mu \text{ but } x_2^2 \text{ does} \} = \{ x_1 x_2 x_3, x_1 x_2^2 x_3, x_1^2 x_3, x_2 x_3^2 \},$
$S_3 = \{ x^\mu : |\mu| = d, x_1^3, x_2^2 \text{ do not divide } x^\mu \text{ but } x_3^3 \text{ does} \} = \{ x_1 x_2 x_3^2, x_1 x_3, x_2 x_3, x_3^3 \}.$

There are clearly \( \binom{d + 2}{2} = 15 \) monomials $x^\mu$ with $|\mu| = d$ and each belongs to one of sets $S_1$, $S_2$, and $S_3$, which are mutually disjoint. Third, we write the system of equations
\[
\begin{cases}
x^\mu / x_1^3 \cdot F_1 = 0 & \text{for all } x^\mu \in S_1, \\
x^\mu / x_2^2 \cdot F_2 = 0 & \text{for all } x^\mu \in S_2, \\
x^\mu / x_3^3 \cdot F_3 = 0 & \text{for all } x^\mu \in S_3.
\end{cases}
\]
Its coefficient matrix in the unknowns $x^\mu$ with $|\mu| = d$,
\[
D = \begin{pmatrix}
-\alpha_2 & 2\alpha_0 & \alpha_2 & -2(1 + \beta_3) \\
-\alpha_2 & 2\alpha_0 & \alpha_2 & -2(1 + \beta_3) \\
-\alpha_2 & 2\alpha_0 & \alpha_2 & -2(1 + \beta_3) \\
\beta_3 & 2\alpha_0 & -1 - \beta_3 \\
\beta_3 & 2\alpha_0 & -1 - \beta_3 \\
\beta_3 & 2\alpha_0 & -1 - \beta_3 \\
-2\alpha_2 & 2\beta_3 & -2\alpha_2 & 2\beta_3 \\
-2\alpha_2 & 2\beta_3 & -2\alpha_2 & 2\beta_3 \\
-2\alpha_2 & 2\beta_3 & -2\alpha_2 & 2\beta_3
\end{pmatrix}.
\]
has the important property that
\[ \text{det}(D) = \text{Res}(Ax^2) \cdot \text{extraneous factor}. \]

Fourth, we turn to consider the extraneous factor. A monomial \( x^v \) of total degree \( d = 4 \) is reduced if \( x_i^2 \) divides \( x^v \) for exactly one \( i \). Let \( D' \) be the submatrix of \( D \) obtained by deleting all rows and columns corresponding to reduced monomials, i.e. in our case,
\[
D' = \begin{bmatrix}
-\alpha_2 & -\alpha_2 & \alpha_2 \\
\beta_3 & -1 - \beta_3 & \alpha_2 \\
\end{bmatrix}.
\]
The extraneous factor is exactly the determinant of \( D' \). Finally, by theorem 4.9 in chapter 3 of [5], to within a sign, the resultant reads as
\[
\text{Res}(Ax^2) = \frac{\text{det} D}{\text{det} D'}
\]
\[
= 16\alpha_2^2(48\alpha_0^2\beta_3 + 4\alpha_0^2(\alpha_2^2 + \beta_3(32\beta_3^2 + 24\beta_3 - 9)) + 3\alpha_0^2(\alpha_2^2(52\beta_3^2 + 28\beta_3 - 1)
\]
\[
+ 4\beta_3^2(8\beta_3^2 + 8\beta_3 - 9\beta_3 - 9)) + 6\alpha_0^2(\alpha_2^2(4\beta_3 + 1) - \alpha_2^2\beta_3(14\beta_3^2 + 36\beta_3 + 35\beta_3
\]
\[
+ 10) - 2\beta_3^2(\beta_3 + 1)(8\beta_3 + 9)) + (\alpha_2^2 - 4(\beta_3 + 1)^2)(\alpha_2^2 - \beta_3^2(2\beta_3 + 3))^2) \tag{12}
\]

**Theorem 4.1 ([5])**. There exists a vector \( x \neq 0 \) such that \( Ax^2 = 0 \) if, and only if, \( \text{Res}(Ax^2) = 0 \), where the formula for \( \text{Res}(Ax^2) \) is given by (12).

By the same approach, we compute the E-characteristic polynomial \( \phi_A(\lambda) \) of the octupolar tensor (9), which is a resultant of the following system of homogeneous polynomial equations
\[
\begin{cases}
\alpha_2 x_1^2 + x_2^2 + x_3^2 - x_0^2 = 0, \\
-\alpha_2 x_1^2 + \alpha_2 x_3^2 + 2\alpha_0 x_3 x_3 - 2(1 + \beta_3)x_2 x_3 - \lambda x_0 x_2 = 0, \\
\beta_3 x_1^2 - (1 + \beta_3)x_2^2 + x_3^2 + 2\alpha_0 x_1 x_2 - \lambda x_0 x_3 = 0, \\
-2\alpha_2 x_1 x_2 + 2\beta_3 x_1 x_3 + 2\alpha_0 x_2 x_3 - \lambda x_0 x_1 = 0.
\end{cases} \tag{13}
\]
Using the software Mathematica, we obtain the E-characteristic polynomial \( \phi_A(\lambda) \).

**Theorem 4.2.** The E-characteristic polynomial of the octupolar tensor (9) is

\[
\phi_A(\lambda) = (\lambda^2 - 1) \sum_{i=0}^{6} c_i \lambda^{2i},
\]

where, in particular,

\[
c_0 = 256\alpha_0^2(48\alpha_0^8\beta_3 + 4\alpha_0^6(\alpha_2^2 + \beta_3(32\beta_3^3 + 24\beta_3 - 9)) + 3\alpha_0^3(52\beta_3^3 + 28\beta_3 - 1)
\]
\[
+ 4\beta_3(8\beta_3^3 + 8\beta_3^3 - 9\beta_3 - 9)) + 6\alpha_0^2(\alpha_2^2(4\beta_3 + 1) - \alpha_2^3\beta_3(14\beta_3^2 + 36\beta_3 + 35\beta_3 + 10)
\]
\[
- 2\beta_3(\beta_3 + 1)^2(8\beta_3 + 9)) + (\alpha_2^2 - 4(\beta_3 + 1)^3)(\alpha_2^2 - \beta_3^2(2\beta_3 + 1))^2.\]

The E-characteristic polynomial \( \phi_A(\lambda) \) is a polynomial of degree 14, with no odd-degree terms. By comparing the expression of \( c_0 \) and (12), we have the following corollary:

**Corollary 4.3.** The constant term of the E-characteristic polynomial \( \phi_A(\lambda) \) is

\[c_0 = [\text{Res}(Ax^2)]^2.\]

This corollary is in agreement with theorem 3.5 of [10] in this case.

**Corollary 4.4.** If \( \text{Res}(Ax^2) \neq 0 \), then all E-eigenvalues of the octupolar tensor \( A \) are non-zero.

**Proof.** Since \( \text{Res}(Ax^2) \neq 0 \), the system \( Ax^2 = 0 \) has only the trivial solution by theorem 4.1. Let us compute \( \phi_A(0) = [\text{Res}(Ax^2)]^2 > 0 \). By theorem 3.7, \( \lambda = 0 \) is not an E-eigenvalue of \( A \).

\[\square\]

5. Octupolar potential

In this section we show how the methods of algebraic geometry recalled in the preceding section afford an explicit algebraic characterization of the critical points of the octupolar potential.

5.1. Dome: the reduced admissible region

We now assume that the North pole \((0, 0, 1)^T\) is the global maximum point of the octupolar potential \( \Phi(x) \) on the unit sphere \( S^2 \). That is, we assume that the octupolar tensor \( A \) has the largest Z-eigenvalue \( \lambda = 1 \) with \((0, 0, 1)^T\) as associated Z-eigenvector. In the admissible region (8), there is a reduced region such that the maximal Z-eigenvalue of \( A \) is 1. The boundary of this reduced admissible region is called the *dome* [7]: its apex is at \( a_0 = 0, \beta_3 = -1/2, \alpha_2 = \frac{\sqrt{2}}{2} \), and it meets the plane \( \alpha_2 = 0 \) along the circle \( \alpha_0^2 + \beta_3^2 + \beta_3 = 0 \).

Now, we are in a position to give an explicit formula for the dome. We consider the E-characteristic polynomial \( \phi_A(\lambda) \) in theorem 4.2. Clearly, \( \lambda = 1 \) is a root of \( \phi_A(\lambda) \). Since the dome is the locus where the maximal Z-eigenvalue is \( \lambda = 1 \), we substitute \( \lambda = 1 \) into \( \phi_A(\lambda)/(\lambda - 1) = 0 \) and we obtain the following equation

\[2c_1(a_0, \beta_3, \alpha_2)^3 \cdot c_2(a_0, \beta_3, \alpha_2) \cdot c_3(a_0, \beta_3, \alpha_2) = 0, \tag{14}\]
where

\[ c_1(\alpha_0, \beta_3, \alpha_2) = 3 - 4\alpha_0^2 - 4\beta_3^2 - 4\beta_3, \quad (15a) \]

\[ c_2(\alpha_0, \beta_3, \alpha_2) = 64\alpha_2^4 - 16\alpha_0^2(1 + 2\beta_3)(-12\alpha_0^2 + (1 + 2\beta_3)^2) + (4\alpha_0^2 + (1 + 2\beta_3)^2)^3, \quad (15b) \]

and

\[ c_3(\alpha_0, \beta_3, \alpha_2) = \alpha_2^2(2\beta_3 - 1)(2\beta_3 + 5)^2 - 12\alpha_0^2 + \alpha_2^4(-48\alpha_0^2(3\beta_3^2 - 1) + 12\alpha_0^2(8\beta_3^2 + 24\beta_3^2 + 26\beta_3^2 - 4\beta_3 - 11) - 16\beta_3^2 - 96\beta_3^2 - 168\beta_3^2 - 72\beta_3^2 - 21\beta_3^2 - 24\beta_3 + 40) + 8\alpha_2^2(8\alpha_0^2 + 6\alpha_0^4(4\beta_3^2 + 2\beta_3 - 5) + 3\alpha_0(8\beta_3^2 + 8\beta_3^2 - 12\beta_3^2 - 3\beta_3 + 6) + 8\beta_3^2 + 36\beta_3^2 + 42\beta_3^2 + 3\beta_3^2 - 9\beta_3^2 - 2) - 16(\alpha_0^2 + \beta_3^2 + \beta_3)^2(4\alpha_0^2 + 4\beta_3^2 + 4\beta_3 - 3), \quad (15c) \]

Because of (8), we know that \( c_1(\alpha_0, \beta_3, \alpha_2) \geq 0 \) and the equality holds on the boundary of the admissible region. Hence, \( c_1(\alpha_0, \beta_3, \alpha_2) = 0 \) is a trivial solution of (14).

As for \( c_2(\alpha_0, \beta_3, \alpha_2) \), this is a quadratic function in \( \alpha_2^2 \) which attains its minimum value \( 4\alpha_0^2(4\alpha_2^2 - 3(1 + 2\beta_3)^2)^2 \geq 0 \). If \( \alpha_0 = 0 \), then \( c_2(\alpha_0, \beta_3, \alpha_2) = (-8\alpha_2^2 + (1 + 2\beta_3)^2)^2 \). Hence, when

\[ \alpha_0 = 0 \quad \text{and} \quad 8\alpha_2^2 - (1 + 2\beta_3)^2 = 0, \quad (16) \]

we have \( c_2(\alpha_0, \beta_3, \alpha_2) = 0 \). If \( 4\alpha_0^2 - 3(1 + 2\beta_3)^2 = 0 \), then \( c_2 = 64(\alpha_2^2 + (1 + 2\beta_3)^2)^2 \). Hence, when

\[ 4\alpha_0^2 - 3(1 + 2\beta_3)^2 = 0 \quad \text{and} \quad \alpha_2^2 + (1 + 2\beta_3)^2 = 0, \quad (17) \]

we also have \( c_2(\alpha_0, \beta_3, \alpha_2) = 0 \).

This is how far we could go with our algebraic analysis: given the complexity of equations (15b) and (15c), our search could be advanced further only with the aid of some explicit numerical probing. In either cases (16) or (17), there are two E-eigenvectors corresponding to the E-eigenvalue 1. One is the North pole \((0, 0, 1)^T\) and the other was always a complex vector in our direct numerical explorations. Hence, we shall disregard the loci \( c_1 = 0 \) and \( c_2 = 0 \).

We now turn attention to the equation \( c_3(\alpha_0, \beta_3, \alpha_2) = 0 \), which has multiple roots in \( \alpha_2 \) for fixed \( \alpha_0 \) and \( \beta_3 \). For example, when \( \alpha_0 = 0 \) and \( \beta_3 = -\frac{4}{\sqrt{3}} \), \( \alpha_2^{(1)} = \alpha_2^{(2)} = -\frac{2}{\sqrt{11}} \approx 0.4851 \) and \( \alpha_2^{(3)} = \frac{4\sqrt{3}}{\sqrt{11}} \approx 0.9466 \) are roots of the equation, whereas when \( \alpha_0 = \frac{1}{\sqrt{58}} \) and \( \beta_3 = -\frac{8}{\sqrt{27}} \), the roots are \( \alpha_2^{(1)} \approx 0.3765, \alpha_2^{(2)} \approx 0.5862 \), and \( \alpha_2^{(3)} \approx 9.459 \). A criterion then need to be devised that identifies which value of \( \alpha_2 \) actually lies on the dome. If the largest Z-eigenvalue of \( A(\alpha_0, \beta_3, \alpha_2) \) is larger that 1, then the triple \( (\alpha_0, \beta_3, \alpha_2) \) is above the dome. Again by direct numerical explorations, we found that, for given \( \alpha_0 \) and \( \beta_3 \), the dome is the continuous surface specified by the smallest non-negative value of \( \alpha_2 \) such that \( c_3(\alpha_0, \beta_3, \alpha_2) = 0 \), i.e.

\[ \alpha_2^{(\text{dome})}(\alpha_0, \beta_3) = \min \{ \alpha_2 \geq 0 : c_3(\alpha_0, \beta_3, \alpha_2) = 0 \} \quad \text{for} \quad \alpha_0^2 + \beta_3^2 + \beta_3 \leq 0, \quad (18) \]

Though some numerical probing was required to arrive at (18), this criterion identifies the dome exactly, if not explicitly. The contour profile of the dome as given by (18) is illustrated in figure 3.

Finally, we say more about the apex and the base of the dome. At the apex of the dome \( (\alpha_0, \beta_3, \alpha_2) = (0, -\frac{1}{\sqrt{2}}, \frac{\sqrt{2}}{2}) \) and the E-characteristic polynomial of the octupolar tensor \( A(0, -\frac{1}{\sqrt{2}}, \frac{\sqrt{2}}{2}) \) is \( \phi_A(\lambda) = 19.683\lambda^6(\lambda^2 - 1)^4 \). There is a quadruple root \( \lambda^2 = 1 \) of such a polynomial associated with four Z-eigenvectors.
\[ \mathbf{x}^{(1)} = (0, 0, 1)^T, \mathbf{x}^{(2)} = \left( \frac{2 \sqrt{3}}{3}, -\frac{1}{3} \right)^T, \mathbf{x}^{(3)} = \left( \frac{\sqrt{6}}{3}, -\frac{\sqrt{2}}{3}, -\frac{1}{3} \right)^T, \mathbf{x}^{(4)} = \left( -\frac{\sqrt{6}}{3}, -\frac{\sqrt{2}}{3}, -\frac{1}{3} \right)^T. \]

The corresponding polar plot of the octupolar potential \( \Phi(\mathbf{x}) \) is precisely that illustrated in figure 2(a).

At the base of the dome, \( \alpha_2 = 0 \) and \( \alpha_0^2 + \beta_3^2 + \beta_3 = 0 \), which represents a circle of center in \( \alpha_0 = 0 \), \( \beta_3 = \frac{1}{2} \) and radius \( \frac{1}{2} \); there, the E-characteristic polynomial reduces to \( \phi_E(\lambda) = -64 \lambda^3 (\lambda^2 - 1)^3 \). Hence, \( \lambda^2 = 1 \) is a triple root of \( \phi_E(\lambda) \). Specifically, \( \mathbf{A}(0, 0, 0) \) has three \( Z \)-eigenvectors, namely,

\[ \mathbf{x}^{(1)} = (0, 0, 1)^T, \mathbf{x}^{(2)} = \left( 0, \frac{\sqrt{3}}{2}, -\frac{1}{2} \right)^T, \mathbf{x}^{(3)} = \left( 0, -\frac{\sqrt{3}}{2}, -\frac{1}{2} \right)^T, \]

associated with the positive \( Z \)-eigenvalue \( \lambda = 1 \). The polar plot of the octupolar potential \( \Phi(\mathbf{x}) \) corresponding to this case is that shown in figure 2(b). As proved in [7], all generic states can be obtained by distorting the plots in figure 2 without changing the number of their maxima.

5.2. Separatrix: the divide between phases

Gaeta and Virga [7] showed by numerical continuation that there is a separatrix surface between the two different generic states of the octupolar potential \( \Phi \): in one generic state, \( \Phi \) has four maxima and three (positive) saddles; in the other generic state, \( \Phi \) has three maxima and two (positive) saddles. Here, we determine explicitly the separatrix.

We recall the octupolar potential \( \Phi(\mathbf{x}) \) defined on the unit sphere \( S^2 \) and note that the normal eigenvalue of the Hessian \( \nabla^2_S \Phi(\mathbf{x}) \) is zero. When passing through the separatrix, two maxima of the octupolar potential \( \Phi(\mathbf{x}) \) on the unit sphere \( S^2 \) coincide. Hence, the product of the two tangential eigenvalues of the Hessian \( \nabla^2_T \Phi(\mathbf{x}) \) must vanish. According to appendix E of [7], this product is equal to

\[ 7 \lambda^2 - 4 \left( (\alpha_0^2 + \alpha_3^2 + \beta_3^2) x_1^2 + (\alpha_0^2 + \alpha_3^2 + (\beta_3 + 1)^2) x_2^2 + (\alpha_0^2 + \beta_3^2 + \beta_3 + 1) x_3^2 \right) - 2 \alpha_0 \alpha_2 x_1 x_2 - 2 \alpha_0 \alpha_2 x_1 x_3 - \alpha_2 \beta_3 x_2 x_3 = 0. \tag{19} \]

Moreover, if \( \lambda \neq 0 \) and \( \mathbf{x} \neq \mathbf{0} \) satisfy \( \mathbf{Ax}^2 = \lambda \mathbf{x} \), then \( \frac{\lambda}{||x||} \) and \( \frac{1}{||x||} \mathbf{x} \) satisfy (11). Hence, we could omit the spherical constraint \( \mathbf{x}^T \mathbf{x} = 1 \) temporarily and just consider the system of homogeneous polynomial equations (19) and

\[
\begin{align*}
-2 \alpha_0 \alpha_2 x_1 x_2 + 2 \beta_3 x_2 x_3 + 2 \alpha_0 x_2 x_3 - \lambda x_1 &= 0, \\
-\alpha_0 x_1^3 + \alpha_0 \alpha_2 x_2 + 2 \alpha_0 x_1 x_3 - 2 (1 + \beta_3) x_2 x_3 - \lambda x_2 &= 0, \\
\beta_2 x_1^3 - (1 + \beta_3) x_2^2 + x_1^2 + 2 \alpha_0 x_1 x_2 - \lambda x_3 &= 0.
\end{align*}
\tag{20}
\]

Using the approach introduced in section 3, we obtain the resultant of (19) and (20)

\[ \text{Separatrix : } 1792 (4 \alpha_0^2 + 4 \beta_3^2 + 4 \beta_3 - 3)^2 \sum_{i=0}^{8} d_2 (\alpha_0, \beta_3) \alpha_0^{2i} = 0, \tag{21} \]

whose coefficients \( d_2 \) are recorded in appendix for completeness.

\[ ^8 \text{Since } \Phi(\mathbf{x}) \text{ is odd in } \mathbf{x}, \text{ both maxima (and positive saddles) of the octupolar potential are accompanied by an equal number of minima (and negative saddles) in the antipodal positions on the unit sphere.} \]
Below the dome, the contour plot of the separatrix as given by (21) is illustrated in figure 4. This shows a 6-fold symmetry, which confirms equation (39) of Gaeta and Virga [7]. We now contrast the separatrix and the dome represented by (21) and (18) to the same surfaces found numerically in [7]. To this purpose, let
\[ \alpha_0 = \rho \cos \chi \quad \text{and} \quad \beta_3 = -\frac{1}{2} + \rho \sin \chi, \] (22)
with \( \rho \in [0, \frac{1}{2}] \) and \( \chi \in (-\pi, \pi] \). In figure 5, for \( \chi = -\frac{\pi}{2}, -\frac{5\pi}{12}, -\frac{\pi}{4}, -\frac{\pi}{6}, \) and \( -\frac{\pi}{6} \), we illustrate the cross-sections of both the dome and the separatrix, in dash-dot lines and solid lines, respectively. It can be easily seen that figure 5 reproduces closely figure 8 in [7].

It readily follows from (22) and (21) that the separatrix intersects the plane \( \alpha_2 = 0 \) along the circles whose radii are the positive roots of the polynomial
\[ (\rho + 1)^3(2\rho + 1)^4\rho^{10}(2\rho - 1)(\rho - 1)^3, \]
the smallest of which identifies the base of the dome. Apart from the three points shown in figure 4 where the separatrix touches this circle, all other points of the latter do not properly belong to the separatrix, defined as the locus that separates regions with four and three maxima of the octupolar potential, which must be continuous: they will thus be considered as spurious points, and so discarded from the separatrix in the following.

Next, to reduce (21) to a simpler form, we study the special case where we set \( \chi = -\frac{\pi}{2} \) in (22), so as to describe a cross-section of the separatrix that reaches the base of the dome. The equation \( c_3(\alpha_0, \beta_3, \alpha_2) = 0 \) for the dome reduces to
\[ -4(\rho + 1)(2\alpha_2^2 - (1 - \rho)(1 + 2\rho)^2)(\alpha_2^2(\rho - 2) - 2\rho + 1)^2 = 0. \]
Clearly, \( \rho + 1 > 0 \). Because \( (1 - \rho)(1 + 2\rho)^2 \) is monotonically increasing in \( \rho \in [0, \frac{1}{4}] \), we get \( (1 - \rho)(1 + 2\rho)^2 \geq 1 \). Hence, by \( 2\alpha_2^2 - (1 - \rho)(1 + 2\rho)^2 = 0 \) and \( \alpha_2 \geq 0 \), we have
that the region in parameter space where $\alpha_2 \geq \frac{1}{\sqrt{2}}$ lies above the dome. Moreover, from $\alpha_2^2(\rho - 2) - 2\rho + 1 = 0$, we know that for $\chi = -\frac{\pi}{2}$ the cross-section of the dome is the curve

$$
\alpha_{2}^{(\text{dome})}(\rho) = \sqrt{\frac{1 - 2\rho}{2 - \rho}}.
$$

(23)

For $\rho \in \left[0, \frac{1}{2}\right]$, $(1 - \rho)^2(1 + \rho)^3 > 0$. Moreover, $\alpha_2^2 + 4(1 - \rho)(1 - 2\rho) \geq 0$ and equality holds if, and only if, $(\rho, \alpha_2) = (\frac{1}{2}, 0)$. Also, $\alpha_2^4 + \alpha_2^2(6\rho + 4) + \rho^2(2\rho + 1)^2 \geq 0$ and equality holds if, and only if, $(\rho, \alpha_2) = (0, 0)$. From $3(3 - \rho)\alpha_2^2 - 4\rho^2(1 - 2\rho) = 0$, we finally obtain that for $\chi = -\frac{\pi}{2}$ the cross-section of the separatrix is the curve

$$
\alpha_{2}^{(\text{sepa})}(\rho) = \frac{2\rho}{\sqrt{3}} \sqrt{\frac{1 - 2\rho}{3 - \rho}}.
$$

(24)

The curves in (23) and (24) have a common vertical tangent at $\rho = \frac{1}{2}$. Moreover, since

$$
[\alpha_{2}^{(\text{dome})}(\rho)]^2 - [\alpha_{2}^{(\text{sepa})}(\rho)]^2 = \frac{(3 - 2\rho)^2(1 - \rho - 2\rho^2)}{3(2 - \rho)(3 - \rho)} \geq 0
$$

Figure 4. The separatrix below the dome as represented by (21).
in $\rho \in [0, \frac{1}{2}]$ and equality holds if, and only if, $\rho = \frac{1}{2}$, we confirm analytically that for $\chi = -\frac{\pi}{2}$, the separatrix lies below the dome all the way down to its base. This reveals that the green dot in figure 8 of [7] where the sepratrix appeared to emanate from the dome, as close as it happened to be the base, was indeed an artefact of the numerical scheme.

By a similar discussion applied at the case $\chi = -\frac{\pi}{6}$, we also obtain the following curves as representations of the meridian cross-sections of dome and separatrix,

$$\alpha_2^{(dome)}(\rho) = \frac{1 - 2\rho}{\sqrt{2}} \sqrt{1 + \rho}, \quad \alpha_2^{(separ)}(\rho) = \frac{2\rho}{\sqrt{3}} \sqrt{\frac{1 + 2\rho}{3 + \rho}}. \quad (25)$$

They intersect for $(\rho, \alpha_2) = \left(\frac{1}{3}, \frac{\sqrt{2}}{\sqrt{3}}\right)$.

6. Summary

We studied the octupolar tensor arising from liquid crystal science. The resultant and the E-characteristic polynomial of the octupolar tensor were constructed explicitly. Using the resultant theory of algebraic geometry and the E-characteristic polynomial of the spectral theory of tensors, we gave an explicit, algebraic expression for the dome and the separatrix, the two significant surfaces for the representation of the octupolar liquid crystal order in three space dimensions. It would be interesting to apply the same algebraic techniques to higher-rank order tensors (or in higher space dimensions) to see whether the pattern of multi-generic states described explicitly in this paper is indeed a persistent feature.
Appendix. Separatrix coefficients

Below we record the explicit, lengthy expressions that deliver the coefficients \(d_{16}\) of the polynomial in \((21)\) as functions of the parameters \(\alpha_0\) and \(\beta_3:\)

\[d_{16} = 27(-16\alpha_0^6 - 8\alpha_0^3(4\beta_3^2 + 44\beta_3 + 13) - (2\beta_3 - 1)(2\beta_3 + 7)^3),\]

\[d_{14} = -54(128\alpha_0^6 - 16\alpha_0^3(48\beta_3^2 + 78\beta_3 - 29) + 16\alpha_0^3(72\beta_3^4 + 124\beta_3^3 + 190\beta_3^2 - 101\beta_3 - 69) + (2\beta_3 + 7)^3(40\beta_3^3 + 44\beta_3^2 + 62\beta_3 - 47)),\]

\[d_{12} = -9(4096\alpha_0^6 - 128\alpha_0^3(277\beta_3^2 - 92\beta_3 - 55) + 48\alpha_0^3(152\beta_3^4 + 1944\beta_3^3 - 7094\beta_3^2 - 1548\beta_3 + 53) + 8\alpha_0^3(5648\beta_3^6 + 184912\beta_3^5 + 60408\beta_3^4 + 115368\beta_3^3 + 86625\beta_3^2 - 44964\beta_3 - 20640) - 1664\beta_3^6 - 22400\beta_3^5 - 124064\beta_3^4 - 377088\beta_3^3 - 624840\beta_3^2 - 383256\beta_3 - 109994\beta_3^2 + 181940\beta_3 - 17605),\]

\[d_{10} = -2(22528\alpha_0^{10} + 5256\alpha_0^7(800\beta_3^2 + 3620\beta_3 + 599) + 64\alpha_0^5(5440\beta_3^6 - 195290\beta_3^5 - 97221\beta_3^4 - 44476\beta_3^3 + 3875 + 16\alpha_0^3(12800\beta_3^4 + 1073640\beta_3^2 + 283244\beta_3^2 + 2369838\beta_3^2 - 242151\beta_3^2 + 492540\beta_3 - 270455) + 4\alpha_0^3(17920\beta_3^6 - 1188320\beta_3^5 + 6499376\beta_3^4 - 13648368\beta_3^3 - 1019872\beta_3^2 + 1289514\beta_3 + 3579185\beta_3^2 + 123260\beta_3 + 206555) + 3276\beta_3^{10} + 483200\beta_3^8 + 3111744\beta_3^6 + 19640064\beta_3^4 + 19640424\beta_3^2 + 5479324\beta_3^2 - 6109790\beta_3^2 - 3422445\beta_3^2 + 504920\beta_3 + 3560),\]

\[d_8 = 5(4096\alpha_0^{12} - 12288\alpha_0^9(97\beta_3^2 + 88\beta_3 + 44) + 256\alpha_0^6(39921\beta_3^4 + 34176\beta_3^4 + 42870\beta_3^4 + 12132\beta_3 + 1667) - 128\alpha_0^3(141080\beta_3^6 + 419208\beta_3^5 + 389430\beta_3^4 + 516622\beta_3^3 + 15613\beta_3^2 + 10040\beta_3 - 37063) + 48\alpha_0^5(1217268\beta_3^6 + 1023680\beta_3^5 + 1963504\beta_3^4 - 1378192\beta_3^4 + 304390\beta_3^2 - 508976\beta_3^2 + 63582\beta_3^2 - 57076\beta_3 - 52349) - 8\alpha_0^7(149376\beta_3^6 + 1199488\beta_3^4 + 4718496\beta_3^4 + 9599232\beta_3^2 + 9822584\beta_3^2 + 3227448\beta_3^2 - 2548818\beta_3^2 - 2029036\beta_3^2 - 53961\beta_3^2 + 37902\beta_3 - 40196) + (2\beta_3 + 1)^2(10304\beta_3^10 + 154304\beta_3^8 + 911472\beta_3^6 + 2786464\beta_3^4 + 4828732\beta_3^2 + 3895212\beta_3^2 + 22345\beta_3^2 - 155868\beta_3^2 - 352512\beta_3^2 + 13318\beta_3 - 7840)),\]

\[d_6 = 16(28672\alpha_0^{14} - 512\alpha_0^{12}(688\beta_3^4 + 1102\beta_3 + 941) - 128\alpha_0^{10}(9696\beta_3^4 - 40380\beta_3^4 - 33951\beta_3^4 - 20148\beta_3 + 11743) - 160\alpha_0^8(5632\beta_3^6 - 26064\beta_3^5 - 7644\beta_3^4 + 35134\beta_3 - 57181\beta_3^2 - 5046\beta_3^2 + 120149\beta_3^2 - 118284\beta_3 - 29175) + 30\alpha_0^6(577536\beta_3^6 + 1111040\beta_3^5 - 2474880\beta_3^4 - 6705600\beta_3^4 - 341600\beta_3^4 + 9137976\beta_3^2 + 5840100\beta_3^2 - 884330\beta_3^2 - 684765\beta_3^2 + 374580\beta_3^2 + 132449) + a_2(2\beta_3 + 1)^2(80896\beta_3^{10} + 999808\beta_3^8 + 3452640\beta_3^6 + 5398208\beta_3^4 + 3717992\beta_3^2 - 367068\beta_3^2 - 2064016\beta_3^2 - 476875\beta_3^2 + 150774\beta_3^2 + 30796\beta_3 - 25928) - (2\beta_3 + 1)\beta_3^2(2048\beta_3^{10} + 25824\beta_3^8 + 135752\beta_3^6 + 385692\beta_3^4 + 535154\beta_3^2 + 253167\beta_3^2 - 114083\beta_3^2 - 118464\beta_3^2 - 4364\beta_3^2 + 7632\beta_3 + 656).\]
\[ d_4 = 16(-32 768 \alpha_0^{16} + 2048 \alpha_0^{14}(241 \beta_1^2 - 284 \beta_3 - 83) + 256 \alpha_0^{12}(9208 \beta_1^4 - 5384 \beta_3^2 + 6390 \beta_1^2) + 25 496 \beta_3 + 8589) + 128 \alpha_0^{10}(25 680 \beta_1^2 - 32 160 \beta_3^2 + 7368 \beta_1^4 + 257 000 \beta_3^3 + 212 292 \beta_1^2) + 23 286 \beta_1^2 - 10 209) + 80 \alpha_0^{8}(8064 \beta_1^3 - 169 344 \beta_3^2 - 304 224 \beta_1^2 + 311 872 \beta_3^2 + 774 736 \beta_1^2) + 306 928 \beta_3^2 - 61 620 \beta_1^2 - 34 824 \beta_3 + 1209) - 8 \alpha_0^{6}(281 856 \beta_1^3 + 2529 280 \beta_1^3 + 6835 200 \beta_1^3) + 6572 800 \beta_1^3 + 316 800 \beta_3^2 - 2303 424 \beta_1^2 - 174 400 \beta_1^2 + 593 920 \beta_3^2 + 124 725 \beta_1^2 - 2310 \beta_3^3 + 6019) - 2 \alpha_0^4(2 \beta_3^2 + 1)^2(230 144 \beta_1^2 + 1285 120 \beta_1^2 + 3244 032 \beta_1^2 + 430 128 \beta_1^2 + 2583 584 \beta_1^2 + 28 128 \beta_3^2 - 669 240 \beta_1^2 - 261 024 \beta_3^2 + 369 \beta_1^2 + 30 952 \beta_3 - 3232) - 4 \alpha_0^2(2 \beta_3^2 + 1)^4(5408 \beta_1^2 + 10 240 \beta_1^2 - 22 272 \beta_3^2 - 72 224 \beta_1^2 - 83 578 \beta_1^2 - 75 384 \beta_1^2 - 40 635 \beta_1^2 + 8889 \beta_1^2 + 10 338 \beta_1^2 - 2444 \beta_3^2 - 184) + 2(2 \beta_3 + 1)^2(2 \beta_3 + 1)^6(400 \beta_1^2 + 400 \beta_1^2 + 15 408 \beta_1^2 + 16 240 \beta_3^2 - 2449 \beta_1^2 - 6128 \beta_3^2 + 104 \beta_3^2 + 272 \beta_3 + 24), \]

\[ d_2 = -256(\alpha_0^2 + \beta_1^2 + \beta_3)^2(4 \alpha_0^2 + (2 \beta_3 + 1)^2)(64 \alpha_0^2 + 8 \alpha_0^2(32 \beta_3^2 - 112 \beta_3 - 81) + 2 \alpha_0^2(192 \beta_1^2 - 576 \beta_1^2 + 1356 \beta_1^2 - 78 \beta_1^2 + 245) + \alpha_0^2(256 \beta_3^2 + 384 \beta_3^2 - 408 \beta_3^2 - 136 \beta_3^2 + 764 \beta_3^2 + 215 \beta_3 + 62) + (2 \beta_3 + 1)^2(16 \beta_3^2 + 144 \beta_3^2 + 266 \beta_3^2 + 87 \beta_3^2 - 89 \beta_3^2 - 32 \beta_3 + 6)), \]

\[ d_0 = 256(\alpha_0^2 + \beta_1^2 + \beta_3)^4(4 \alpha_0^2 + 4 \beta_1^2 + 4 \beta_3^2 + 3)(4 \alpha_0^2 + (2 \beta_3 + 1)^2)^4. \]

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**References**

[1] Brand H R and Pleiner H 2010 Macroscopic behavior of non-polar tetrahedralematic nematic liquid crystals *Eur. Phys. J. E* 31 37–50

[2] Brand H R, Pleiner H and Cladis P E 2002 Flow properties of the optically isotropic tetrahedral phase *Eur. Phys. J. E* 7 163–6

[3] Buckingham A D 1967 Flow properties of the optically isotropic tetrahedral phase *Eur. Phys. J. E* 7 163–6

[4] Cartwright D and Sturmfels B 2013 The number of eigenvalues of a tensor *Linear Algebra Appl.* 438 942–52

[5] Cox D A, Little J and O’Shea D 2004 *Using Algebraic Geometry* 2nd edn (New York: Springer)

[6] Fei L G 1995 Tetrahedral symmetry in nematic liquid crystals *Phys. Rev. E* 52 702–17

[7] Gaeta G and Virga E G 2016 Octupolar order in three dimensions *Eur. Phys. J. E* 39 113

[8] Jäkli A 2013 Liquid crystals of the twenty-first century—nematic phase of bent-core molecules *Liq. Cryst. Rev. 1* 65–82

[9] Lascat S et al 2007 Discotic liquid crystals: from tailor-made synthesis to plastic electronics *Angew. Chem., Int. Ed.* 46 4832–87

[10] Li A-M, Qi L and Zhang B 2013 E-characteristic polynomials of tensors *Commun. Math. Sci.* 11 33–53

[11] Link D R, Natale G, Shao R, Maclellan J E, Clark N A, Köbrlova E and Walba D M 1997 Spontaneous formation of macroscopic chiral domains in a fluid smectic phase of achiral molecules *Science* 278 1924–7

[12] Liu K, Nissinen J, Slager R-J, Wu K and Zaamen J 2016 Generalized liquid crystals: giant fluctuations and the vestigial chiral order of L, O, and T matter *Phys. Rev. X* 6 041025

[13] Lubensky T C and Radzihovsky L 2002 Theory of bent-core liquid-crystal phases and phase transitions *Phys. Rev. E* 66 031704
[14] Ni G, Qi L, Wang F and Wang Y 2007 The degree of the E-characteristic polynomial of an even order tensor J. Math. Anal. Appl. 329 1218–29
[15] Niori T, Sekine T, Watanabe J, Furukawa T and Takezoe H 1996 Distinct ferroelectric smectic liquid crystals consisting of banana shaped achiral molecules J. Mater. Chem. 6 1231–3
[16] Nissinen J, Liu K, Slager R-J, Wu K and Zaanen J 2016 Classification of point-group-symmetric orientational ordering tensors Phys. Rev. E 94 022701
[17] Onsager L 1949 The effects of shape on the interaction of colloidal particles Ann. New York Acad. Sci. 51 627–59
[18] Palffy-Muhoray P, Pevnyi M, Virga E G and Zheng X 2017 The effects of particle shape in orientationally ordered soft materials Mathematics and Materials (IAS/Park City Mathematics Series vol 23) ed M J Bowick et al (Providence, RI: American Mathematical Society) pp 201–53
[19] Piastra M and Virga E G 2013 Octupolar approximation for the excluded volume of axially symmetric convex bodies Phys. Rev. E 88 032507
[20] Qi L 2005 Eigenvalues of a real supersymmetric tensor J. Symb. Comput. 40 1302–24
[21] Qi L 2007 Eigenvalues and invariants of tensors J. Math. Anal. Appl. 325 1363–77
[22] Qi L and Luo Z 2017 Tensor Analysis: Spectral Theory and Special Tensors (Philadelphia, PA: Society for Industrial and Applied Mathematics)
[23] Romano S 2008 Computer simulation study of a simple tetrahedratic mesogenic lattice model Phys. Rev. E 77 021704
[24] Sonnet A M and Virga E G 2012 Dissipative Ordered Fluids (New York: Springer)
[25] Trojanowski K, Pajak G, Longa L and Wydro T 2012 Tetrahedratic mesophases, chiral order, and helical domains induced by quadrupolar and octupolar interactions Phys. Rev. E 86 011704
[26] Turzi S S 2011 On the Cartesian definition of orientational order parameters J. Math. Phys. 52 053517
[27] Virga E G 2015 Octupolar order in two dimensions Eur. Phys. J. E 38 63
[28] Wiant D, Neupane K, Sharma S, Gleeson J T, Sprunt S, Jakli A, Pradhan N and Iannacchione G 2008 Observation of a possible tetrahedratic phase in a bent-core liquid crystal Phys. Rev. E 77 061701