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On some orthogonality properties of Maxwell's multipole vectors

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Abstract

We determine the location of the expansion points with respect to which the two Maxwell's multipole vectors of the quadrupole moment and the dipole vector of a distribution of charge form an orthogonal trihedron. We find that with respect to these 'orthogonality centres' both the dipole and the quadrupole moments are each characterized by a single real parameter. We further show that the orthogonality centres coincide with the stationary points of the magnitude of the quadrupole moment and, therefore, they can be seen as an extension of the concept of centre of the dipole moment of a neutral system introduced previously in the literature. The nature of the stationary points then provides the means for the classification of a distribution of charge in two different categories.

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1. Introduction

The multipole expansion [1] is a useful tool for the representation of various fields (electromagnetic and gravitational for example) because it allows their resolution in terms of a hierarchical set of symmetry features describing their sources. In most applications the accent is placed on the characterization of the field rather than the source itself and therefore the study of the multipole coefficients is limited to properties that directly relate to how they affect the field. More recent studies however [2–5] show the relevance of these parameters for the characterization of the spatial organization of the source of the field. Therefore, the study of the geometric and symmetry properties of the multipole moments is an interesting problem in itself.

There are two more common ways to discuss the multipolar representations and the relationship between them is non-trivial beyond the lowest orders. In the Cartesian approach the multipole moments are the coefficients of Taylor's expansion of the electrostatic potential

of a distribution of charge about a given point in space [1]. Due to symmetry properties and the fact that the potential satisfies Laplace's equation outside the region occupied by the charge, the Cartesian multipole coefficients of a given expansion order form the components of a totally symmetric and traceless tensor of a rank equal to the order of expansion. These properties make the components of the tensor highly dependent. The enumeration of the independent components is facilitated by the use of irreducible tensorial sets [6] in which the moments are represented in terms of solid spherical harmonics. This second way of describing the multipole moments corresponds to the original formalism of the potential theory developed by Maxwell [7].

Besides providing the means for an irreducible representation, Maxwell's approach has the advantage of exposing geometrical features of the source of a field satisfying Laplace's equation. Indeed, Sylvester's theorem [8, 9] shows that any spherical harmonic function can be characterized by a set of unit vectors (Maxwell's multipole vectors) and a general scalar constant. These parameters are a direct characterization of the spatial organization of the source of the field. The direction in space of Maxwell's multipole vectors can then be used to extract information about the spatial organization of the distribution of various quantities. This is a common technique for the analysis of the level of anisotropy of the cosmic microwave background [3, 4, 10], for example. In other research [2], such geometrical features were implicitly used to define 'canonical' reference frames for the spatial registration of the biological molecules. Our own interest in these aspects emerged from the need for alternative parameterization of the physicochemical properties of large protein structures [5]. This convergence of applications towards geometrical interpretation of the multipole moments motivated us towards the analysis presented in this paper.

To introduce the concepts used throughout the paper, we will consider for the sake of simplicity a discrete system of point-like particles. The results can be straightforwardly extended to the continuous case. The spherical multipole moments of such a system, q_{lm}, are the coefficients of the expansion of the scalar potential in terms of spherical harmonic functions [1] at large distances from the source

$$\Phi(\vec{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{1}{2l+1} \frac{q_{lm}}{r^{l+1}} Y_{lm}(\hat{r}), \tag{1}$$

and are given by the expression

$$q_{lm} = \sum_{i=1}^{N} e_i r_i^l Y_{lm}^*(\hat{r}). \tag{2}$$

The summation runs over all N particles in the system and e_i denotes the scalar property of interest which, for concreteness, will be named charge throughout the paper. In equations (1) and (2) r stands for the length and $\hat{r}$ for the direction (equivalent to a pair of spherical angular coordinates θ, ϕ) of a position vector.

Up to a distance-dependent factor, the sum over m in equation (1) can be expressed as a homogeneous polynomial of order l in the three Cartesian components x, y, z of the vector $\vec{r}$. Therefore, it satisfies Sylvester's theorem [8, 11] which provides a representation in terms of the l Maxwell's multipole vectors and a constant factor [7, 9] in the form

$$r^l \sum_{m=-l}^{l} q_{lm} Y_{lm}(\hat{r}) = C(\hat{u}_1 \cdot \vec{r}) \cdots (\hat{u}_l \cdot \vec{r}) + r^2 \mathcal{F}. \tag{3}$$

Maxwell's unit vectors $\hat{u}_i$ are defined up to an inversion since the sign can be absorbed in the value of the constant C (they are headless vectors). Within this paper we will make the

assumption that the signs are chosen such that the overall constant is positive. The function $\mathcal{F}$ is a homogeneous polynomial of degree $l-2$ in x, y, z and is completely determined by the same set of unit vectors $\hat{u}_i$. Then, equation (3) shows that there exists a one-to-one correspondence between the spherical multipoles q_{lm} on one hand, and the constant C and the set of Maxwell's multipole vectors on the other hand. Maxwell's unit vectors $\hat{u}_i$ and the constant C provide therefore a geometrical description of the source of the field. Throughout this paper we will refer to the vectors $\hat{u}_i$ with the term Maxwell's multipole vectors or just multipole vectors when no confusion may arise.

The set of multipole coefficients of a given rank $\{q_{lm}\}_{m=-l\cdots l}$ form irreducible tensorial sets [6] and therefore they behave as vectors of various dimensions under rotations of the three-dimensional physical space. They are however sensitive to translations and, accordingly, so do their associated Maxwell's multipole vectors. It is meaningful therefore to ask: how does the relative orientation of the multipole vectors depend on the location of the origin of coordinates? While the problem deserves a more general analysis in the context of multipoles of arbitrary order, here we will only focus on the lowest non-trivial orders, i.e. on the relative orientation of Maxwell's dipole and quadrupole moments. More specifically we will define the conditions of orthogonality of the three multipole vectors.

We would like to note that the question we study here is a particular aspect of the more general problem of the translational properties of the multipole moments [2, 12–15]. To our best knowledge, no study exists that approaches these properties in the context of Maxwell's vector representation of the multipole moments (either in electrostatic or a more general context).

The organization of the paper is as follows. In section 2 we derive the expansion points with respect to which the dipole and quadrupole multipoles form an orthogonal trihedron (orthogonality centres). We also show that, with respect to the orthogonality centres, the quadrupole and dipole moments each can be characterized by a single real parameter. In section 3 we outline a method to construct the orthogonal trihedron of the quadrupole and dipole Maxwell's multipole vectors. In section 4 we show that the orthogonality centres are stationary points of the magnitude of the quadrupole moment and discuss their nature. Section 5 concludes the paper.

2. The orthogonality centers

The relative orientation of the two multipole vectors of the quadrupole moment, as well as the relative orientation between any of these vectors and the dipole vector change under the translation of the origin of the reference frame but are invariant with respect to rotations. In general, the angle between two multipole vectors can take any value. In particular, it can be expected that, with respect to certain expansion points, orthogonality between various pairs of multipole vectors, considered independently, can be achieved. There will be however at most three multipole vectors that can be simultaneously pairwise orthogonal, since all vectors reside in the three-dimensional physical space. We will call such an expansion point with respect to which this condition is satisfied an orthogonality centre.

From a simple count of unknowns and equations we can anticipate that points with this property exist. Indeed, there are three independent translation coordinates and three orthogonality conditions. This leads to a set of three constraints for three unknowns which can, at least in principle, be satisfied by an appropriate three-dimensional translation.

Solving the system of constraints defined above can be in principle done directly using one of the methods for derivation of Maxwell's multipoles [4, 9, 16] and then imposing the

orthogonality conditions. This is however a laborious path and here we will use instead an indirect approach.

The relative directions of the three unit vectors of the dipole and quadrupole moments are conveniently represented by three scalar products. As rotational invariants, these scalar products should serve as building blocks for the functional representation of various invariant quantities that can be formed with the dipole and quadrupole moments. By examining these invariants, we will identify the equations that need to be satisfied by the dipole and quadrupole moments, when calculated with respect to the orthogonality centre, so that the orthogonality conditions of their multipole vectors hold.

Since the desired orthogonality conditions involve both dipole and quadrupole moments, we will seek invariants involving both sets of coefficients. Constructing such invariants is governed by the general theory of irreducible tensor operators [17, 18]. The lowest rank tensor resulting from the coupling of the quadrupole (rank 2) and dipole (rank 1) moments is a regular three-dimensional (rank 1) vector. The components of this vector are

$$a_\mu = [\mathbf{q}_2 \times \mathbf{q}_1]_{1\mu}, \tag{4}$$

where the symbol $[\cdots \times \cdots]$ stands for tensor coupling and $\mathbf{q}_2$ and $\mathbf{q}_1$ denote respectively the sets of components of the quadrupole and dipole moments. The index μ takes one of the three values denoting the spherical components of the vectors, i.e. -1, 0, $+1$.

The components a_μ can be expressed in terms of individual components of the coupled tensors using the appropriate Clebsch–Gordan coefficients [17, 18] $C^{211}_{\mu_2\mu_1\mu}$ as

$$a_\mu = \sum_{\mu_2=-2}^{2} \sum_{\mu_1=-1}^{1} C^{211}_{\mu_2\mu_1\mu} q_{2\mu_2} q_{1\mu_1}. \tag{5}$$

The coefficients $C^{211}_{\mu_2\mu_1\mu}$ are readily available in textbooks [17] or can be calculated with a scientific software [19]. After substituting their values, the set of equations (5) becomes

$$a^{\mathrm{re}}_{11} = \sqrt{\tfrac{3}{10}}\big(q^{\mathrm{re}}_{22} p_x - q^{\mathrm{im}}_{22} p_y - q^{\mathrm{re}}_{21} p_z - \tfrac{1}{\sqrt{6}} q_{20} p_x\big), \tag{6}$$

$$a^{\mathrm{im}}_{11} = \sqrt{\tfrac{3}{10}}\big(q^{\mathrm{im}}_{22} p_x + q^{\mathrm{re}}_{22} p_y - q^{\mathrm{im}}_{21} p_z + \tfrac{1}{\sqrt{6}} q_{20} p_y\big), \tag{7}$$

$$a_{10} = \sqrt{\tfrac{3}{5}}\big(q^{\mathrm{re}}_{21} p_x - q^{\mathrm{im}}_{21} p_y - \sqrt{\tfrac{2}{3}} q_{20} p_z\big). \tag{8}$$

For convenience, in these equations the components of the quadrupole and of the resulting vector a are expressed in terms of their real and imaginary parts, and the dipole components are converted to their Cartesian form defined by $p_x = -\sqrt{2} q^{\mathrm{re}}_{11}$, $p_y = \sqrt{2} q^{\mathrm{im}}_{11}$, $p_z = q_{10}$.

To derive the functional form of vector a in terms of Maxwell's multipole vectors, we use equation (15) of [4] to express the quadrupole moments in terms of their multipole unit vectors. To avoid unnecessary clutter, we do not enforce the normalization of Maxwell's vectors. Instead, we assume that the general multiplication constant in equation (3) is absorbed symmetrically in the vectors defining the multipole moments. When applied to quadrupole moments, the equations read

$$q^{\mathrm{re}}_{22} = \sqrt{\frac{3}{40\pi}}(u_{1x} u_{2x} - u_{1y} u_{2y}), \tag{9}$$

$$q^{\mathrm{im}}_{22} = -\sqrt{\frac{3}{40\pi}}(u_{1x} u_{2y} + u_{1y} u_{2x}), \tag{10}$$

$$q_{21}^{\mathrm{re}} = -\sqrt{\frac{3}{40\pi}}(u_{1x}u_{1z} + u_{1z}u_{2x}), \tag{11}$$

$$q_{21}^{\mathrm{im}} = \sqrt{\frac{3}{40\pi}}(u_{1y}u_{1z} + u_{1z}u_{2y}), \tag{12}$$

$$q_{20} = \sqrt{\frac{1}{5\pi}}u_{1z}u_{2z} - \sqrt{\frac{1}{20\pi}}(u_{1x}u_{2x} + u_{1y}u_{2y}). \tag{13}$$

Maxwell's multipole unit vector for the dipole moment coincides with its direction. The only invariant associated with vector a is its length. After substituting the above expressions for the components of the quadrupole moment in equations (6)–(8), the length of vector a becomes

$$\|a\|^2 = 2\left(a_{11}^{\mathrm{re}}\right)^2 + 2\left(a_{11}^{\mathrm{im}}\right)^2 + a_{20}^2 \tag{14}$$

$$= \frac{1}{200\pi}\left[9u_1^2(\vec{p}\cdot\vec{u}_2) + 9u_2^2(\vec{p}\cdot\vec{u}_1) + 4p^2(\vec{u}_1\cdot\vec{u}_2) - 6(\vec{u}_1\cdot\vec{u}_2)(\vec{p}\cdot\vec{u}_1)(\vec{p}\cdot\vec{u}_1)\right]. \tag{15}$$

Equation (15) shows that the orthogonality conditions $\vec{u}_1\cdot\vec{u}_2 = \vec{u}_1\cdot\vec{p} = \vec{u}_2\cdot\vec{p} = 0$ require that the length of vector a is zero. From equation (14) it then follows that

$$a_{11}^{\mathrm{re}} = a_{11}^{\mathrm{im}} = a_{20} = 0. \tag{16}$$

This is the implicit form of the necessary set of equations that need to be satisfied by the quadrupole and dipole multipole vectors so that they form a set of three orthogonal directions.

Equations (9)–(13) can also be exploited to extract the angle between the quadrupole multipole vectors. By calculating the magnitude of the quadrupole vector $\|q_2\|^2 = [\mathbf{q}_2\times\mathbf{q}_2]_{00} = \sum_m q_{2m}^* q_{2m}$, we find

$$(\vec{u}_1\cdot\vec{u}_2)^2 = 20\pi\|q_2\|^2 - 3u_1^2u_2^2. \tag{17}$$

Then, used together, equations (14), (15) and (17) provide means for further analysis of the relative orientation of any pair of the three Maxwell's multipole vectors in terms of the quadrupole and dipole components.

A more meaningful form of equation (16) results when these conditions are expressed in terms of the quadrupole Cartesian components. Then the set of equations (16) becomes

$$\mathcal{Q}\vec{p} = 0. \tag{18}$$

The matrix $\mathcal{Q}$ represents, up to a factor of $1/3$, the traceless Cartesian quadrupole tensor defined by

$$\mathcal{Q} = \mathcal{S} - (1/3)\ \mathrm{Tr}(\mathcal{S})\mathbf{1}_3, \tag{19}$$

$$\mathcal{S}_{\alpha\beta} = \sum_{i=1}^{N} e_i r_{i\alpha} r_{i\beta}, \tag{20}$$

where $\mathbf{1}_3$ is the identity matrix in the three-dimensional space and $r_{i\alpha}$ denotes the three Cartesian components of the position vector of particle i. For the derivation of equation (18), the spherical quadrupole moments were expressed in terms of their Cartesian components as [1] $q_{20} = 3/4\sqrt{5/\pi}\,\mathcal{Q}_{33}$, $q_{21}^{\mathrm{re}} = -1/2\sqrt{15/2\pi}\,\mathcal{Q}_{13}$, $q_{21}^{\mathrm{im}} = 1/2\sqrt{15/2\pi}\,\mathcal{Q}_{23}$, $q_{22}^{\mathrm{re}} = 1/2\sqrt{15/2\pi}(\mathcal{Q}_{11} + 1/2\mathcal{Q}_{33})$, $q_{22}^{\mathrm{im}} = -1/2\sqrt{15/2\pi}\,\mathcal{Q}_{12}$.

Equation (18) shows that, with respect to an orthogonality centre, the dipole moment needs to be an eigenvector of the matrix of the quadrupole tensor corresponding to a zero

eigenvalue. When the dependence on the expansion centre is made explicit, this equation will determine the origin with respect to which the orthogonality conditions are satisfied.

Note that equation (18) also implies that, with respect to an orthogonality centre, both the quadrupole and the dipole moments are each characterized by a single real parameter. Indeed, since the Cartesian quadrupole matrix is traceless and one of its eigenvalues vanishes, the remaining eigenvalues are equal in absolute value and of opposite sign. Then, their common absolute value is sufficient to characterize the quadrupole moment. In particular, the magnitude of the quadrupole moment is proportional to this parameter. At the same time, the dipole moment has a direction implied by its orientation along the eigenvector of null eigenvalue. Thus, the only parameter needed to fully describe the dipole is its magnitude.

Before further exploring the result, let us note that equation (18) coincides formally with the equation of the 'centre of the dipole moment' as defined in [2, 20]. In that context, a neutral system is assumed. For neutral systems, the centre of the charge is not defined and the dipole moment is invariant with respect to the expansion centre [1]. In the absence of a centre of charge, a 'centre of the dipole moment' is sought to serve as a standard origin for a multipolar representation. The 'centre of the dipole moment' is defined in [2] from a condition of 'minimal quadrupole contribution' to the electrostatic potential. We see here that the 'centre of the dipole moment' has also a geometric interpretation of representing the point where the three multipole vectors, one for the dipole and two for the quadrupole moment, form an orthogonal trihedron. Since the dipole moment $\vec{p}$ does not depend on the centre of expansion in this case, and the net charge of the system is zero (which removes terms quadratic in the translation vector in the Cartesian quadrupole as will be shown below), equation (18) is linear in the position of the expansion centre and therefore it yields a unique 'centre of the dipole'. We consider in this paper the general case of a non-neutral system, and, as we will see later, this leads to a more complex equation for the centre(s) of orthogonality. Since the (unique) centre of orthogonality coincides in the neutral case with the 'centre of the dipole moment', and since this quantity is derived in detail in [2], we will not discuss this particular case here.

The dependence of the spherical quadrupole moments on the centre of expansion can be made explicit from their laws of transformation under translation. General equations exist for arbitrary orders (see for example [12]). For our purpose, it is more convenient to use instead the obvious transformation of the Cartesian quadrupole and dipole moments, which requires the substitutions $\mathcal{S}_{\alpha\beta} \to \mathcal{S}_{\alpha\beta} - r_\alpha \mathcal{P}_\beta - r_\beta \mathcal{P}_\alpha + q r_\alpha r_\beta$, and $\vec{p} \to \vec{\mathcal{P}} - q\vec{r}$. The vector $\vec{r} = (x, y, z)$ is the position of the centre of expansion, $\vec{\mathcal{P}} = \sum_{i=1}^{N} e_i \vec{r}_i$ is the dipole moment vector with respect to the original (arbitrary) origin and q is the total charge of the system. Then, with respect to an arbitrary origin, the spherical quadrupole moments are expressed as

$$q_{22}^{\mathrm{re}} = \frac{1}{4}\sqrt{\frac{15}{2\pi}}(\mathcal{S}_{xx} - \mathcal{S}_{yy} - 2x\mathcal{P}_x + 2y\mathcal{P}_y + qx^2 - qy^2), \tag{21}$$

$$q_{22}^{\mathrm{im}} = -\frac{1}{2}\sqrt{\frac{15}{2\pi}}(\mathcal{S}_{xy} - x\mathcal{P}_y - y\mathcal{P}_x + qxy), \tag{22}$$

$$q_{21}^{\mathrm{re}} = -\frac{1}{2}\sqrt{\frac{15}{2\pi}}(\mathcal{S}_{xz} - x\mathcal{P}_z - z\mathcal{P}_x + qxz), \tag{23}$$

$$q_{21}^{\mathrm{im}} = \frac{1}{2}\sqrt{\frac{15}{2\pi}}(\mathcal{S}_{yz} - y\mathcal{P}_z - z\mathcal{P}_y + qyz), \tag{24}$$

$$q_{20} = \frac{1}{2}\sqrt{\frac{5}{4\pi}}(3\mathcal{S}_{zz} - \mathrm{Tr}(\mathcal{S}) - 6z\mathcal{P}_z + 2\vec{r}\cdot\vec{\mathcal{P}} + 3qz^2 - qr^2). \tag{25}$$

Substituting all these results back in equations (6)–(8) and then using equation (16), we arrive at the desired equation for the centre of orthogonality. It is convenient to express the result in terms of the position of the orthogonality centre with respect to the centre of charge, i.e. in terms of the vector $\vec{R} = \vec{r} - \vec{\mathcal{P}}/q$, because this vector is invariant to translation (as the direction between two points rigidly tied to the structure). Hence, the equation reads

$$\left(\mathcal{D} - \tfrac{1}{3}\,\mathrm{Tr}(\mathcal{D})\mathbf{1}_3\right)\vec{R} = -\tfrac{2}{3}qR^2\vec{R}, \tag{26}$$

with $\mathcal{D}$ being the matrix

$$\mathcal{D} = \mathcal{S} - \frac{1}{q}\vec{\mathcal{P}}\vec{\mathcal{P}}. \tag{27}$$

Alternatively, this result could have been obtained directly from equation (18) with the transformation outlined above for the Cartesian quadrupole and dipole moments.

We note that the second term in equation (27) represents, up to a constant, the direct product of the centre of the charge, $\vec{\mathcal{P}}/q$, with itself. For a charged system ($q \neq 0$) this quantity is always defined and by shifting the origin of the calculation at this location, the term disappears from equation. This leads to

$$\mathcal{Q}_c\vec{R} = -\tfrac{2}{3}qR^2\vec{R}, \tag{28}$$

where $\mathcal{Q}_c$ is 1/3 of the traceless quadrupole tensor with respect to the centre of charge.

Equation (28) has the appearance of an eigenvector–eigenvalue problem with $-(2/3)qR^2$ playing the role of the eigenvalue. Obviously, equation (28) admits the trivial solution $\vec{R} = 0$. This solution represents the centre of charge where $\|a\|^2 = 0$ because the dipole moment vanishes at that location, and therefore it does not represent a real orthogonality centre.

To further discuss equation (28), let us assume that the net charge is positive. For nontrivial solutions, we need then to select from among the negative eigenvalues of the matrix $\mathcal{Q}_c$. Since $\mathcal{Q}_c$ is a three-dimensional traceless matrix, it has at least one and at most two negative eigenvalues. Then, each negative eigenvalue determines two orthogonality centres located oppositely with respect to the centre of charge along the direction of the corresponding eigenvector. If λ is such a negative eigenvalue, then the coordinates of the two corresponding orthogonality centres, $\vec{R}_{\mathrm{oc}}$, are

$$\vec{R}_{\mathrm{oc}} = \pm\sqrt{3\lambda/2}\hat{v}, \tag{29}$$

where $\hat{v}$ is the normalized eigenvector corresponding to eigenvalue λ.

3. The orthogonal trihedron of the multipole vectors

The construction of the orthogonal multipole trihedron at an orthogonality centre can be done by directly calculating Maxwell's multipole vectors of the dipole and quadrupole moments. Calculating the dipole vector is trivial since it reduces to the position of the centre of charge with respect to the orthogonality centre. For the calculation of the quadrupole multipole vectors, a numerical scheme such as the ones described in [4, 9, 16] can be used.

Alternatively, Maxwell's multipole vectors can be calculated from the eigenvectors of the Cartesian quadrupole moment. According to equation (18), the dipole moment is the eigenvector of the Cartesian tensor corresponding to the null eigenvalue. When calculated with respect to an orthogonality centre the quadrupole multipole vectors are perpendicular to the dipole, and therefore they reside in the plane of the other two eigenvectors of the Cartesian quadrupole tensor, i.e. of the eigenvectors corresponding to the non-zero (one positive and one negative) eigenvalues. This is a particular case of a more general property that the quadrupole multipole vectors are always in the plane spanned by the two eigenvectors corresponding

to the maximum and the minimum eigenvalues of the Cartesian quadrupole tensor. Indeed, it has been shown [21] that these two eigenvectors can be obtained as the following linear combinations:

$$\hat{a}_{\pm} = (\hat{u} \pm \hat{v})/\|\hat{u} \pm \hat{v}\|, \tag{30}$$

of the multipole vectors $\hat{u}, \hat{v}$. The two normalized eigenvectors $\hat{a}_{\pm}$ correspond to the largest and smallest eigenvalues

$$\lambda_{\pm} = \frac{C}{5}\left(\frac{1}{3}\hat{u} \cdot \hat{v} \pm 1\right). \tag{31}$$

The third eigenvector is therefore perpendicular to the plane determined by $\hat{u}, \hat{v}$ and is associated with an eigenvalue

$$\lambda_0 = -\frac{C}{15}\hat{u} \cdot \hat{v}. \tag{32}$$

The multipole vectors $\hat{u}, \hat{v}$ can be obtained by solving the system of equation (30). This can be reduced to a linear system by observing that the denominator on the right-hand side can be expressed in terms of $\hat{u} \cdot \hat{v}$ only. This quantity and the constant C can be found simultaneously by solving equations (31) and (32), and this leads to

$$C = \frac{5}{2}(\lambda_+ - \lambda_-), \tag{33}$$

$$\hat{u} \cdot \hat{v} = -\frac{3\lambda_0}{\lambda_+ - \lambda_-}. \tag{34}$$

Then, if we define $\cos(\alpha) = \hat{u} \cdot \hat{v}$, simple trigonometrical manipulations yield

$$\|\hat{u} + \hat{v}\| = 2\cos(\alpha/2), \tag{35}$$

$$\|\hat{u} - \hat{v}\| = 2\sin(\alpha/2). \tag{36}$$

The solution of equation (30) is then expressed as

$$\hat{u} = \hat{a}_+ \cos(\alpha/2) + \hat{a}_- \sin(\alpha/2), \tag{37}$$

$$\hat{v} = \hat{a}_+ \cos(\alpha/2) - \hat{a}_- \sin(\alpha/2). \tag{38}$$

At the position of an orthogonality centre $\lambda_0 = 0$ and, therefore, $\alpha = \pi/2$. Then, the multipole vectors are parallel to the two diagonals of the square formed by the eigenvectors $\hat{a}_{\pm}$, i.e.

$$\hat{u} = (1/\sqrt{2})(\hat{a}_+ + \hat{a}_-), \tag{39}$$

$$\hat{v} = (1/\sqrt{2})(\hat{a}_+ - \hat{a}_-). \tag{40}$$

4. Orthogonality centres as stationary points of the quadrupole moment

As discussed in section 2, equation (18) is formally equivalent to the equation defining the centre of the dipole moment of a neutral system [2]. Since in that context the equation is obtained from a condition of minimum of the magnitude of the quadrupole moment with respect to translations, it is useful to explore to what extent that condition applies to this more general case of a charged systems.

The magnitude of the quadrupole moment relates to the Cartesian components as

$$\sum_m |q_{2m}|^2 = \frac{15}{8\pi} \sum_{\alpha\beta} Q_{\alpha\beta}^2. \tag{41}$$

Under a translation of vector $\vec{r}$, the Cartesian components change as

$$Q'_{\alpha\beta} = Q_{\alpha\beta} - r_\alpha p_\beta - r_\beta p_\alpha + (2/3)\vec{r}\cdot\vec{p}\delta_{\alpha\beta} + q r_\alpha r_\beta - (1/3) q r^2 \delta_{\alpha\beta}. \tag{42}$$

The extremes of the magnitude of the quadrupole moment are reached when its gradient vanishes. This requires

$$\frac{\partial}{\partial r_\gamma} \sum_{\alpha\beta} |Q'_{\alpha\beta}|^2 = \sum_{\alpha\beta} Q'_{\alpha\beta} \frac{\partial Q'_{\alpha\beta}}{\partial r_\gamma} = 0, \qquad \gamma = 1, 2, 3. \tag{43}$$

The derivatives of $Q'_{\alpha\beta}$ can be easily calculated from equation (42) and they read

$$\begin{aligned} \frac{\partial Q'_{\alpha\beta}}{\partial r_\gamma} &= -p_\beta \delta_{\alpha\gamma} - p_\alpha \delta_{\beta\gamma} + \frac{2}{3} p_\gamma \delta_{\alpha\beta} - \frac{2}{3} q r_\gamma \delta_{\alpha\beta} + q r_\alpha \delta_{\beta\gamma} + q r_\beta \delta_{\alpha\gamma} \\ &= -(p_\beta - q r_\beta)\delta_{\alpha\gamma} - (p_\alpha - q r_\alpha)\delta_{\beta\gamma} + \frac{2}{3}(p_\gamma - q r_\gamma)\delta_{\alpha\beta}. \end{aligned} \tag{44}$$

The last term in equation (44) makes no contribution under the summation in equation (43) because of the traceless character of the quadrupole matrix. The other two terms are proportional to the components of the dipole moment at the translated point, p'_α. Substituting these remaining terms back into equation (43) leads to $Q'\vec{p}' = 0$, i.e. the same equation as (18).

To establish the nature of the stationary points, we calculate the Hessian of the squared quadrupole magnitude at these points. The result can be easily interpreted if we use a system of axes placed at the stationary point and with orientation along the eigenvectors of the Cartesian quadrupole. This choice renders the Hessian diagonal and it now reads

$$H = \begin{pmatrix} \frac{4}{3}p^2 & 0 & 0 \\ 0 & \frac{2}{3}(p^2 + q\mu) & 0 \\ 0 & 0 & \frac{2}{3}(p^2 - q\mu) \end{pmatrix}, \tag{45}$$

where μ and $-\mu$ are the only non-zero eigenvalues of the quadrupole tensor at the stationary point and p represents the magnitude of the dipole moment at the same location. It is obvious that at least two eigenvalues of the Hessian are positive. Therefore, the orthogonality centre is either a minimum or a saddle point. The nature of the stationary point is determined by the signs of the two diagonal elements $p^2 \pm q\mu$. If $p^2 \geqslant |q\mu|$, both values are positive and therefore the point is a point of minimum. In the alternative case, only one of the eigenvalues is positive and therefore the point is a saddle point.

As shown earlier, the orthogonality centres come in pairs of points located symmetrically from the centre of charge along each axis of negative eigenvalue. Only the magnitude of the dipole moment appears in the Hessian (equation (45)), and therefore both centres in a given pair have the same nature, either both of them are points of minimum or both of them are saddle points. It is easy to establish that for a given system, there cannot be more than one pair of minima. Indeed, the dipole moment with respect to a given orthogonality centre is $p^2 = q^2R^2 = -(3/2)q\lambda_1$, where λ_1 is a negative eigenvalue (with respect to the centre of charge) with which the centre is associated. On the other hand, by using equation (42) to relate translated eigenvalues, one finds that $\mu = \pm(\lambda_2 - qR^2/3)$, the $\pm$ sign depending on which of the two remaining eigenvalues is represented by λ_2. Then, one can find that the condition of minimum, $p^2 \geqslant |q\mu|$, requires $\lambda_1 \leqslant \lambda_2 \leqslant -2\lambda_1$. One can see that the left side of the

inequality cannot be satisfied when the role of the two eigenvalues is interchanged. Therefore, even if both eigenvalues are negative and, therefore, they both have associated orthogonality centres, only one of the pairs of centres forms minima, and that pair corresponds to the negative eigenvalue of the maximum absolute value. The other pair is necessarily a saddle point.

Note that the right-hand side inequality is always satisfied due to the traceless property satisfied by the three quadrupole eigenvalues. Assume the three eigenvalues are ordered as $\lambda_1 \leqslant \lambda_2 \leqslant \lambda_3$. Then, $\lambda_3 = -\lambda_1 - \lambda_2 \leqslant -\lambda_1 - \lambda_1 = -2\lambda_1$ and since λ_3 is the maximum of the three eigenvalues, this proves the property.

To summarize, the above analysis shows that there always exists a pair of orthogonality centres which are at the same time points of minima of the quadrupole moment with respect to translations. These orthogonality centres correspond to the negative eigenvalue with maximum absolute value of the Cartesian quadrupole (with respect to the centre of charge). When more than one negative eigenvalue exists, a second pair of orthogonality centres exists and those centres are saddle points for the quadrupole moment. These two categories of charge conformations can also be succinctly described by the two parameters p—the dipole moment, and μ—the quadrupole moment corresponding to a point of minimum of the quadrupole moment: for $p^2 \geqslant |q\mu|$, the quadrupole moment has two saddle points with respect to the translation of the physical system, in addition to the two minima; for $p^2 \in (\min\{-q\mu, q\mu\}, \max\{-q\mu, q\mu\})$, there are no saddle points.

5. Conclusions

In this paper we show that there are locations in space (orthogonality centres) with respect to which Maxwell's vectors of the quadrupole and dipole moments form an orthogonal trihedron. We prove that the orthogonality centres are located symmetrically along the principal axes of negative eigenvalues of the Cartesian quadrupole matrix with respect to the centre of charge. There are two orthogonality centres for each negative eigenvalue, and their distances to the centre of charge are expressed in terms of the eigenvalues of the Cartesian quadrupole with respect to the centre of charge.

With respect to an orthogonality centre, the quadrupole and dipole moments are each characterized by a single parameter. The orthogonality centres represent stationary points of the magnitude of the quadrupole moment with respect to three-dimensional translations. The nature of the stationary points depends on the relative magnitude of the dipole and quadrupole moments with respect to those points. Then, the three-dimensional landscape of a distribution of charge can be characterized at the quadrupole level on the basis of the relative magnitude of these parameters at the point of minimum of the quadrupole moment.

The relationship between the orthogonality centres and the stationary points of the magnitude of the quadrupole moment suggests a possible path towards the extension of the notion of centres to higher order multipoles. In general, such centres cannot be defined by orthogonality properties since for arbitrary higher orders the number of Maxwell's vectors exceeds the dimensionality of the space. However, the condition of stationarity admits generalization to any multipolar order. This path has been briefly explored before [2] as a means to define the centre of the quadrupole moment for the particular case of a system with zero net charge and zero overall electric dipole.

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