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Note

A Computational Procedure for Obtaining the Poles of a Spherical Harmonic of Order N; Application to the Multipole Expansion of Electrostatic Interaction*

The solution for the poles of a general spherical surface harmonic is analyzed with application to the multipole calculation for the interaction of two charge distributions. The theoretical advantages are discussed and have been verified in test calculations using a FORTRAN program available on request.

1. Introduction

The energy of the electrostatic interaction of two nonoverlapping charge distributions A and B can be written as a double Taylor series of $1/|\mathbf{r}_B - \mathbf{r}_A|$ about the two origins $\mathbf{O}_A$ and $\mathbf{O}_B$ in the following notation, which is convenient for subsequent use:

$$E_{AB} = \sum_{N=0}^{\infty} \sum_{N_A=0}^{N} E_{N_A, N_B}, \qquad N_B = N - N_A, \tag{1}$$

where

$$E_{N_A,N_B} = \sum_{\{\mathbf{n}_A, \mathbf{n}_B\}} I_A(\mathbf{n}_A) * I_B(\mathbf{n}_B) * \prod_{i=1}^{N_A} (\mathbf{s}_i(\mathbf{n}_A) \cdot \nabla_A) * \prod_{i=1}^{N_B} (\mathbf{s}_i(\mathbf{n}_B) \cdot \nabla_B)(1/(|\mathbf{r}_B - \mathbf{r}_A|))\Big|_{\mathbf{r}_\gamma = \mathbf{O}_\gamma}, \tag{2}$$

$$\nabla_\gamma = \sum_{i=1}^{3} \mathbf{e}_i(\partial/\partial x_{\gamma i})$$
$$I_\gamma(\mathbf{n}_\gamma) = \int \rho_\gamma \prod_{i=1}^{3} x_i^{n_{\gamma i}}\, d\mathbf{x} \Big/ \prod_{i=1}^{3} n_{\gamma i}!\,, \tag{3}$$

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$$\begin{aligned} \mathbf{s}_i(\mathbf{n}_\gamma) &= \mathbf{e}_1 , & 1 \leqslant i \leqslant n_{\gamma 1} \\ &= \mathbf{e}_2 , & n_{\gamma 1} + 1 \leqslant i \leqslant n_{\gamma 1} + n_{\gamma 2} \\ &= \mathbf{e}_3 , & n_{\gamma 1} + n_{\gamma 2} + 1 \leqslant i \leqslant n_{\gamma 1} + n_{\gamma 2} + n_{\gamma 3} = N_\gamma \\ & & (\gamma = A \text{ or } B, i = 1,..., N_\gamma), \end{aligned} \tag{4}$$

where ρ_γ is the charge density of system γ and the $\hat{e}_i$ defines an orthogonal right-handed basis set. The expression for E_{N_A,N_B} is of the form [1]

$$E_{N_A,N_B} = |\mathbf{x}|^{-2(N_A+N_B)-1} * Y_{N_A,N_B}(\mathbf{x}), \tag{5}$$

$$Y_{N_A,N_B}(\mathbf{x}) = \sum_{\{\mathbf{n}_A,\mathbf{n}_B\}} c(\mathbf{n}_A , \mathbf{n}_B) \prod_{i=1}^{3} x_i^{n_{Ai}+n_{Bi}}, \tag{6}$$

where $\mathbf{x} = \mathbf{O}_B - \mathbf{O}_A$, Y_{N_A,N_B} is a homogeneous polynomial of degree $N_A + N_B$, and E_{N_A,N_B} satisfies Laplace's equation and is, therefore, a spherical harmonic as defined by Hobson [2a]. Thus, the theorem establishing the existence of unique real poles can be applied.[1] It follows, that for each center and for each N_A , N_B there exists a unique set of real pole vectors (characteristic directions) $\mathbf{s}_1^{N_A},..., \mathbf{s}_{N_A}^{N_A}$, $\mathbf{s}_1^{N_B},..., \mathbf{s}_{N_B}^{N_B}$ and multipole moments $p_A^{(N_A)}$, $p_B^{(N_B)}$ such that the sum of directional derivatives in Eq. (2) can be replaced by one directional derivative:

$$\begin{aligned} E_{N_A,N_B} = &\{p_A^{(N_A)} * p_B^{(N_B)}/(N_A! * N_B!)\} \\ &* \prod_{i=1}^{N_A} (\mathbf{s}_i^{N_A} \cdot \nabla_A) * \prod_{i=1}^{N_B} (\mathbf{s}_i^{N_B} \cdot \nabla)(1/(|\mathbf{r}_B - \mathbf{r}_A|))\Big|_{\mathbf{r}_\gamma=\mathbf{O}_\gamma} . \end{aligned} \tag{7}$$

Clearly, these characteristic directions and multipole moments are determined by $E_{N_A,0}$ and E_{0,N_B} .

Since in general, Eq. (2) is a sum of $(N_A + 1)(N_A + 2)(N_B + 1)(N_B + 2)/4$ directional derivatives, it is more efficient to use Eq. (7) to obtain E_{N_A,N_B} than to use Eq. (2). It will be shown that the solution for the characteristic directions and multipole moments of Eq. (7) and the calculation of E_{AB} by Eqs. (1) and (7) involves approximately the same computer time as the calculation of E_{AB} by Eqs. (1) and (2) for one orientation, and becomes overwhelmingly advantageous as the number of orientations for the same charge distributions increases.

An added advantage of the form (7) for a spherical harmonic and of writing Eq. (2) as a sum of terms that are special cases of the form (7) lies in the fact

[1] Hobson [2 Theorem 8, Eq. (9), p. 127] gives the result for any spherical harmonic $Y_n(x, y, z)$: $Y_n(\partial/\partial x, \partial/\partial y, \partial/\partial z)(1/r) = (-1)^n((2n)!/2^n n!)(1/r^{2n+1}) Y_n(x, y, z)$. On page 135 he shows that the Y_n on the right-hand side is not unique and proceeds to show on page 135 ff. that the pair of equations $Y_n(x, y, z) = 0$, $x^2 + y^2 + z^2 = 0$ defines a unique set of real poles.

that it leads naturally to an extension where the inclusion of the induced moments involves the same computational procedure [3].

In Sections 2 and 3, the procedure to obtain the poles and multipole moments of any spherical harmonic of order N will be described, and in Section 4, the application of this procedure to $E_{N_A,0}$ will be presented.

2. Determination of the Poles of a Spherical Harmonic

It has been shown [2b], that if $|\mathbf{x}|^{-2N-1} * Y_N(\mathbf{x})$ is a spherical harmonic of order N, then the ith pole will be given by (the asterisk stands for the complex conjugate)

$$\mathbf{s}_i = \mathbf{v}_i / |\mathbf{v}_i|, \qquad \mathbf{v}_i = \begin{vmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 \\ x_1{}^i & x_2{}^i & x_3{}^i \\ x_1^{i*} & x_2^{i*} & x_3^{i*} \end{vmatrix}, \tag{8}$$

where $(x_1{}^i, x_2{}^i, x_3{}^i)$ is the ith simultaneous root of the equations

$$Y_N(\mathbf{x}) = 0, \tag{9}$$

$$\sum_{i=1}^{3} x_i{}^2 = 0. \tag{10}$$

In general, Eq. (9) can be written in the form

$$Y_N'(\mathbf{x}) = x_3 Y_{N-1}''(\mathbf{x}), \tag{11a}$$

$$Y_N'(\mathbf{x}),\ Y_{N-1}''(\mathbf{x}), \qquad \text{polynomials of degrees } N,\ N-1, \text{ respectively, of even order in } x_3. \tag{11b}$$

It is convenient to eliminate x_3 from Eq. (11) by Eq. (10) in order to replace the pair of equations by a single equation, a homogeneous polynomial in x_1, x_2, in a fashion to be described:

$$P_M(x_1, x_2) = \sum_{i=0}^{M} c_i x_1{}^i x_2^{M-i} = 0. \tag{12}$$

Three cases are considered:

Case even–odd. Neither Y_N' nor $Y_{N-1}'' \equiv 0$. Each side of Eq. (11) is squared and the roots of the resulting equation:

$$P_M(x_1, x_2) = (Y_N'(x_1, x_2, x_3(x_1, x_2)))^2 - (x_3(x_1, x_2))^2\,(Y_{N-1}''(x_1, x_2, x_3(x_1, x_2)))^2, \qquad M = 2N, \tag{13}$$

are to be found.

Case even. $Y''_{N-1} \equiv 0$. In this case

$$P_M(x_1, x_2) = Y_N(x_1, x_2, x_3(x_1, x_2)), \qquad M = N. \tag{14}$$

This case always arises whenever the system has a symmetry plane and $\mathbf{e}_3$ is chosen perpendicular to it.

Case odd. $Y_N' \equiv 0$. In this case, there is a root for which $x_3 = 0$ and

$$P_M(x_1, x_2) = Y''_{N-1}(x_1, x_2, x_3(x_1, x_2)), \qquad M = N - 1. \tag{15}$$

The following step will require the separation of the trivial roots of P_M of the form

$$(x_1, 0) \text{ and } (0, x_2), \qquad x_1, x_2 \neq 0, \text{ otherwise arbitrary}. \tag{16}$$

These will be present if and only if there exist positive j_1 and/or j_2 such that $c_j = 0$ if $j < j_1$ and/or if $M - j < j_2$. In these cases $(0, x_2)$ will be a j_1-fold and/or $(x_1, 0)$ will be a j_2-fold root of P_M.

Consider, therefore, the reduced equation of order $M - j_1 - j_2$:

$$P_M^r(x_1, x_2) = \sum_{i=0}^{M'} c_{i+j_1} * x_1{}^i * x_2^{M'-i} = 0 \qquad (M' = M - j_1 - j_2). \tag{17}$$

Since $P_M{}^r$ is homogeneous and there are no roots of the form (16), it follows that if (x_1, x_2) is a root then $x_1, x_2 \neq 0$ and (x_1, x_2) are determined only up to a ratio. Therefore, set $x_2 = 1$ and solve for the roots of

$$P_M^{r'}(x_1) = \sum_{i=0}^{M'} c_{i+j_1} * x_1{}^i, \qquad (M' = M - j_1 - j_2), \tag{18}$$

to obtain the roots of P_M not of the form (16).

It follows from Eq. (10) that every root (x_1, x_2) of P_M yields

$$x_3 = \pm(-x_1{}^2 - x_2{}^2)^{1/2}. \tag{19}$$

The conditions under which each root of P_M yields a unique set of conjugate roots or 2 sets,

$$\begin{aligned} &\{(x_1, x_2, +(-x_1{}^2 - x_2{}^2)^{1/2}), (x_1{}^*, x_2{}^*, +(-x_1{}^2 - x_2{}^2)^{1/2*})\}, \\ &\{(x_1, x_2, -(-x_1{}^2 - x_2{}^2)^{1/2}), (x_1{}^*, x_2{}^*, -(-x_1{}^2 - x_2{}^2)^{1/2*})\}, \end{aligned} \tag{20}$$

will now be discussed.

In case even–odd, it is necessary to select from (20) those roots that are roots of Eqs. (9) and (10), since the solution of $P_M = 0$ will introduce roots that are not roots of Eqs. (9) and (10).

A simple lemma is proved first:

LEMMA. *If* (x_1, x_2) *is a root of* P_M *of Eq.* (13) *and* $(x_1, x_2, \pm x_3(x_1, x_2))$ *are both r-fold roots of Eq.* (9), *or equivalently,* (11) *and* $x_3(x_1, x_2) \neq 0$, *then* (x_1, x_2) *is a* $2r$*-fold root of* P_M.

Proof. Y_N' and Y''_{N-1} are both invariant upon a change in sign of x_3. But $Y_N' = x_3 Y''_{N-1}$ can be invariant only if $Y_N' = 0$. Since $x_3 \neq 0$, $Y''_{N-1} = 0$. It follows, that (x_1, x_2) must be an r-fold root of Y_N' and Y''_{N-1}, and thus, a $2r$-fold root of $P_M = (Y_N')^2 - x_3(x_1, x_2)^2 * (Y''_{N-1})^2$.

Remark. If x_1, x_2 are both real, this always is the case since then x_3 must be pure imaginary, thus, $(x_1, x_2, x_3)^* = (x_1, x_2, -x_3)$.

The following cases will be considered:

1. $x_3 = 0$. In this case there is a unique set of conjugate roots: $(x_1, x_2, 0)$, $(x_1^*, x_2^*, 0)$.

2. $x_3 \neq 0$; (x_1, x_2) real. According to the remark, (x_1, x_2) is a $2r$-fold root of P_M, but $(x_1, x_2, x_3(x_1, x_2))$ is only an r-fold root of Eq. (11). Therefore, it is necessary to discard r of the $2r$ occurrences. Note that since (x_1, x_2) is only determined up to a ratio, x_1, x_2 in the trivial case (16) can always be chosen as real.

3. $x_3 \neq 0$; (x_1, x_2) complex. Then, it is necessary to substitute one of the conjugates from each of the two sets of (20) into Eq. (9) with the following two possible results:

(a) One root of P_M must be rejected since it fails to satisfy Eq. (9).

(b) Both sets satisfy Eq. (9). It follows from the Lemma that (x_1, x_2) is a $2r$-fold root of P_M and that r of these occurrences must be removed.

In case even and case odd, there is no squaring, which can introduce false occurrence of roots. However, if (x_1, x_2) is real, the use of Eq. (19) would yield two identical sets in (20). Therefore, only one set has to be generated.

3. Determination of the Multipole Moments

The multipole moments can be obtained by the equation

$$p^{(N)} = |\mathbf{x}_0|^{-2N-1} * Y_N(\mathbf{x}_0) \Big/ \left\{ \prod_{i=1}^{N} (\mathbf{s}_i \cdot \nabla)(1/|\mathbf{x}|) \Big|_{\mathbf{x}=\mathbf{x}_0} \Big/ N! \right\}, \tag{21}$$

where the value of $\mathbf{x}_0$ is chosen arbitrarily.

Since $p^{(N)}$ should be independent of the choice of $\mathbf{x}_0$, by computing $p^{(N)}$ at more than one choice of $\mathbf{x}_0$, a consistency check is obtained on the poles.

4. The Explicit Form of Equations (9) and (10) for $E_{N_A,0}$

If the spherical harmonic in question is $E_{N_A,0}$, the expansion of the directional derivatives according to [1, Eq. (10)] shows that $E_{N_A,0}$ of Eq. (2) is a linear combination of products of the $(\mathbf{s}_i \cdot \mathbf{x})$ and/or the $(\mathbf{s}_i \cdot \mathbf{s}_j)$. Use of [1, Eq. (14)] shows that $|\mathbf{x}|^{2N_A+1} * E_{N_A,0}$ is a homogeneous polynomial in which the only term not containing $|\mathbf{x}|^2$ as a factor is

$$\prod_{l=1}^{N_A} [-(2l-1)] * \prod_{k=1}^{N_A} (\mathbf{s}_k \cdot \mathbf{x}). \tag{22}$$

From Eqs. (2), (4), (22), it follows that the Eq. (9) $E_{N_A,0} = |\mathbf{x}|^{-2N-1} Y_N(\mathbf{x}) = 0$ can be replaced by the simpler

$$\sum_{\{\mathbf{n}_A\}} I_A(\mathbf{n}_A) * \prod_{i=1}^{3} x_i^{n_{Ai}} = 0, \tag{23a}$$

$$I_A(\mathbf{n}_A), \qquad \text{cf., Eq. (3).} \tag{23b}$$

Clearly, in the calculation of $p^{(N)}$, the $Y_N(\mathbf{x}_0)$ cannot be simplified as in the calculation of the characteristic directions by Eqs. (10) and (23).

5. Discussion

The procedure to obtain the poles and multipole moments of a surface spherical harmonic of order N has been analyzed in detail and its application to the problem of the multipole expansion of electrostatic interaction has been given.

The polar formalism has the advantage that it permits an extension to the problem of the interaction of polarizable charge distributions within the framework of the same formalism [3].

The proposed procedure has the following advantage. Since in absence of zero integrals Eq. (2) has $(N_A + 1) * (N_A + 2) * (N_B + 1) * (N_B + 2)/4$ terms, the use of Eq. (2) requires approximately $N_A^2 * N_B^2/4$ times more similar calculations than Eq. (7). This is increased when it is extended to the induced moment problem.

The only added work required by the new procedure is the following single calculation to obtain the characteristic directions and multipole moments:

(i) the solution for the complex roots of a polynomial of degree N or $2N$ (depending on whether the charge distribution has a symmetry plane or not);

(ii) the evaluation of $E_{N,0}$ by Eq. (2).

A CDC FORTRAN program of the above procedure has been written and is available on request. As a check on its accuracy, the characteristic directions and multipole moments of four point charges located at the four vertices of a tetrahedron were computed up to order 10.

It was found that:

1. The multipole moments computed at different choices of $\mathbf{x}_0$ agreed at least in nine-decimal digits;

2. The E_{AB} value computed by Eqs. (1) and (7) and the E_{AB} value computed by the Coulomb law (at distances great enough to expect convergence with $N \leqslant 10$) agreed to seven- to nine-decimal digits, depending on the orientation. The discrepancy of two-decimal digits is accounted for the loss of figures through subtraction in the Coulomb calculation;

3. The computation of all the characteristic directions and multipole moments up to order 10 took 7.8 sec on a CDC 6600 computer; the computation of E_{AB} (using only E_{N_A,N_B} with $N_A + N_B \leqslant 10$) with Eq. (7) took 0.65 sec, using Eq. (2) it took 6.6 sec. Thus, even with the high symmetry of the tetrahedron, the time requirement decreased by a factor of 10 and the new procedure altogether took about the same time even when the generated characteristic directions and multipole moments were used only once.

References

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