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Traceless cartesian tensor forms for spherical harmonic functions: new theorems and applications to electrostatics of dielectric media

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Abstract. A solid spherical harmonic of degree n at a point $\boldsymbol{r}$ takes the tensor contraction form $\mathbf{A}^{(n)}\cdot n\cdot \boldsymbol{r}^n$, where $\mathbf{A}^{(n)}$ is a totally symmetric and traceless nth-rank cartesian tensor. The utility of this form rests on the properties of a detracer operator $\mathscr{T}_n$ which transforms any totally symmetric nth-rank tensor to a totally traceless form. In particular, the components of the tensor $\mathscr{T}_n\boldsymbol{r}^n$, which is related to the nth gradient of r^{-1}, are spherical harmonics with properties analogous to those of the tesseral harmonics $Y_n^m(\theta, \phi)$, including adherence to an addition theorem and an 'Unsöld' theorem. These properties lead to new formulae for the Legendre polynomials and their derivatives in terms of cartesian tensors. The traceless cartesian tensor forms are used to treat problems in electrostatics of a dielectric medium requiring spherical harmonic expansions of the potential. These include the potentials arising from an arbitrary charge distribution in a spherical dielectric cavity, the reaction field gradients in the cavity, the response of a dielectric sphere embedded in a dielectric medium to an arbitrary external field, and the gradients of the Lorentz internal field in a homogeneous dielectric. Expressions are obtained for nth-order field gradients and induced multipole moments in cartesian tensor form.

1. Introduction

A function $f(x, y, z)$ of the cartesian coordinates is called a solid spherical harmonic of degree n if f is homogeneous of degree n in x, y, z and satisfies the Laplace equation $\nabla^2 f = 0$. These functions occur widely in physics in such diverse problems as potential theory, hydrodynamics, conduction of heat and sound, diffusion, wave motion, and the quantum theory of angular momentum (MacRobert 1947, Margenau and Murphy 1956, Sommerfeld 1949, Edmonds 1974).

This paper is concerned with some new methods of treating spherical harmonics in cartesian form. The methods are based on certain connections between spherical harmonics of degree n and traceless cartesian tensors of rank (or order) n. Two such connections are touched upon in the literature and will be developed here: (i) if a traceless tensor of rank n is independent of x, y, z, then its components serve as the constant coefficients in a spherical harmonic of degree n (MacRobert 1947, p134); and (ii) there is a class of traceless tensors of rank n whose components are themselves nth-degree spherical harmonic functions of x, y, z (Gray and Gubbins 1984, p493). A simple example will illustrate both of these connections. The function

$$f = 2x^2 - y^2 - z^2 \tag{1.1}$$

is a solid spherical harmonic of degree 2. The constant coefficients $2, -1, -1$ comprise a diagonal tensor of rank 2, and their sum vanishes. Furthermore, the function in (1.1) is one of a set of functions which together constitute a traceless cartesian tensor of rank 2. These functions, referred to here as cartesian basis spherical harmonics, are closely related to the gradient tensor $\nabla\nabla r^{-1}$.

Traditional treatments of physical problems involving spherical harmonics usually employ the spherical polar coordinates r, θ, ϕ and use as basis functions the tesseral harmonics, which are related to the associated Legendre functions $P_n^m(\cos\theta)$. For example, (1.1) is equivalent to

$$f = r^2[\tfrac{1}{2}P_2^2(\cos\theta)\cos 2\phi - P_2^0(\cos\theta)]$$

where each term on the right is itself a solid spherical harmonic of degree 2. Similarly, any potential function which obeys the Laplace equation can be expanded in terms of the tesseral harmonics (Böttcher 1952, p469). When this is done, the coefficients of the spherical basis functions comprise *spherical* tensor forms for physical quantities of interest, such as multipole moments of charge distributions or gradients of the potential at some origin. A major aim of the present work is to provide an analogous spherical harmonic formalism in which the coefficients of the basis functions used in an expansion comprise *cartesian* tensor forms for the physical quantities of interest. The formalism is used here to solve a number of problems in the electrostatics of dielectric media containing embedded spheres or spherical cavities. These yield several higher-order relationships which, to the best of my knowledge, have not been obtained previously by either spherical or cartesian tensor methods.

The connections between cartesian and spherical tensors and their relative merits for various problems have been discussed by Stone (1975, 1976) and by Gray and Gubbins (1984). For our purposes it may be noted that nth-rank symmetric and traceless cartesian tensors are equivalent to nth-rank spherical tensors, in that both have $2n+1$ independent components and are related to each other by a linear transformation. The cartesian tensor forms for multipole moments and potential gradients have the conceptual advantage of being straightforward extensions of one-dimensional moments and gradients, and they have the practical advantage of being easily incorporated into electromagnetic theory in the conventional cartesian form. It would appear that the reason cartesian tensors have not been more widely used in spherical harmonic theory is that the procedure for obtaining the symmetric and traceless part of an nth-rank tensor has not been well understood. This procedure is expressed in the present work by means of an operator $\mathscr{T}_n$ (the 'detracer'), which takes a number of explicit forms. Most of the results obtained here follow from the special properties of the detracer, which have been partially demonstrated elsewhere (Applequist 1984) and are developed more fully here.

In what follows, §§ 2–4 deal with background in tensor notation and the basic properties of tensor contraction forms for homogeneous polynomials and spherical harmonics. Section 5 develops some forms of the detracer operator and its properties. Sections 6 and 7 relate the cartesian basis spherical harmonics to the gradients of r^{-1} and to the Legendre polynomials. Section 8 is a collection of further matters concerning the cartesian basis spherical harmonics, including relations for gradients and integrals, linearly independent subsets, relations to tesseral harmonics, and particular values of the functions. Section 9 treats the electrostatic potentials of an arbitrary charge distribution in a dielectric cavity, including the nth-order potential gradients, using primarily the principles in §§ 5–7. Section 10 uses similar methods to treat the electrostatics of a dielectric sphere embedded in a dielectric medium, including the field gradients and induced multipole moments in the sphere, with special attention given to the Lorentz internal field and its gradients.

2. Notation

2.1. *Tensors*

A cartesian tensor of rank n will be denoted either by a boldface sans-serif symbol $\mathsf{A}^{(n)}$ or by the component notation $A^{(n)}_{\alpha_1\ldots\alpha_n}$, following the convention that Greek subscripts denote cartesian axes $1, 2, 3$ (corresponding to x, y, z respectively). The complete tensor is an array of 3^n components. If $A^{(n)}_{\alpha_1\ldots\alpha_n}$ is invariant under any permutation of the sequence $\alpha_1 \ldots \alpha_n$, the tensor is said to be totally symmetric. The compressed form of a totally symmetric tensor $\mathsf{A}^{(n)}$ is an array of the $(n+1)(n+2)/2$ independent components of $\mathsf{A}^{(n)}$. It will sometimes be convenient to represent the components of the compressed tensor by $A^{(n)}(n_1n_2n_3)$, where n_i is the number of times i occurs in the index set $\alpha_1 \ldots \alpha_n$, and $n_1 + n_2 + n_3 = n$. The components of the polyadic tensor $\boldsymbol{r}^n$, where $\boldsymbol{r}$ is a position vector, may thus be written $r_{\alpha_1} \ldots r_{\alpha_n}$ or $x^{n_1}y^{n_2}z^{n_3}$.

2.2. *Tensor contractions*

An n-fold contraction will be indicated by $\cdot\, n\, \cdot$, as in

$$\mathsf{A}^{(n)} \cdot n \cdot \mathsf{B}^{(n)} = A^{(n)}_{\alpha_1\ldots\alpha_n} B^{(n)}_{\alpha_n\ldots\alpha_1}$$

where the convention of implied summation over repeated Greek subscripts is followed. For totally symmetric tensors, the contraction may be expressed in terms of the compressed forms by (Applequist 1983)

$$\mathsf{A}^{(n)} \cdot n \cdot \mathsf{B}^{(n)} = \sum_{n_1n_2n_3} g(n; n_1n_2n_3) A^{(n)}(n_1n_2n_3) B^{(n)}(n_1n_2n_3) \tag{2.1}$$

where

$$g(n; n_1n_2n_3) = n!/n_1!n_2!n_3!$$

and the sum in (2.1) is over all non-negative indices such that $n_1 + n_2 + n_3 = n$.

2.3. *Traces*

The trace of $\mathsf{A}^{(n)}$ in one index pair is denoted by

$$A^{(n:1)}_{\alpha_3\ldots\alpha_n} = A^{(n)}_{\nu\nu\alpha_3\ldots\alpha_n}$$

a tensor of rank $n-2$. If the trace vanishes regardless of which index pair is contracted, the tensor is said to be totally traceless. A totally symmetric tensor which is traceless in one index pair is traceless in all index pairs, and is said to be totally symmetric and traceless. In compressed tensor notation, the trace can be written

$$A^{(n:1)}(n_1n_2n_3) = A^{(n)}(n_1 + 2, n_2, n_3) + A^{(n)}(n_1, n_2 + 2, n_3) + A^{(n)}(n_1, n_2, n_3 + 2) \tag{2.2}$$

where $n_1 + n_2 + n_3 = n - 2$. The trace of $\mathbf{A}^{(n)}$ in m index pairs, called an 'm-fold trace', is written

$$A^{(n:m)}_{\alpha_{2m+1}\ldots\alpha_n} = A^{(n)}_{\nu_1\nu_1\ldots\nu_m\nu_m\alpha_{2m+1}\ldots\alpha_n} \tag{2.3}$$

a tensor of rank $n - 2m$. In the present work we will be concerned with m-fold traces of only totally symmetric tensors, so the notation of (2.3) applies to any m-fold trace. In compressed tensor notation, the m-fold trace is

$$A^{(n:m)}(n_1 n_2 n_3) = \sum_{k_1 k_2 k_3} g(m; k_1 k_2 k_3) A^{(n)}(n_1 + 2k_1, n_2 + 2k_2, n_3 + 2k_3) \tag{2.4}$$

where $n_1 + n_2 + n_3 = n - 2m$ and the sum is over all non-negative indices such that $k_1 + k_2 + k_3 = m$. The trinomial coefficient $g(m; k_1 k_2 k_3)$ appears here as the number of ways one can place k_1 pairs 11, k_2 pairs 22, and k_3 pairs 33 in the indices $\nu_1\nu_1 \ldots \nu_m\nu_m$ of the m-fold trace.

3. Homogeneous polynomials

3.1. Tensor contraction lemma

Let $\boldsymbol{r}$ be the cartesian vector (x, y, z), and let $\boldsymbol{r}^n$ be the direct product of the n vectors $\boldsymbol{r}$, a cartesian tensor of rank n. Let $h_n(\boldsymbol{r})$ be a polynomial in x, y, z of degree n. The tensor contraction form for homogeneous polynomials, stated in the following lemma, is basic to the present formalism.

Lemma. An nth-degree polynomial $h_n(\boldsymbol{r})$ is homogeneous in x, y, z, of degree n, if and only if

$$h_n(\boldsymbol{r}) = \mathbf{A}^{(n)} \cdot n \cdot \boldsymbol{r}^n \tag{3.1}$$

where $\mathbf{A}^{(n)}$ is a cartesian tensor of rank n, independent of $\boldsymbol{r}$.

Proof. By definition, h_n is homogeneous of degree n if and only if $h_n(t\boldsymbol{r}) = t^n h_n(\boldsymbol{r})$. This condition is met by the right-hand side of (3.1), regardless of whether the set of coefficients $\mathbf{A}^{(n)}$ constitute a tensor. Furthermore, (3.1) includes all possible polynomial terms satisfying this condition. It remains to prove that $\mathbf{A}^{(n)}$ is a tensor, given the form of (3.1). The right-hand side can be regarded as the scalar product of the 3^n-dimensional column vectors $\mathbf{A}^{(n)}$ and $\boldsymbol{r}^n$, and can be written in the matrix form $\mathbf{A}^{(n)\mathrm{T}}\boldsymbol{r}^n$, where T denotes transpose. If we place a second set of cartesian axes, rotated with respect to the original set, into the space of the function, the value of h_n does not change at any point. However, $\boldsymbol{r}^n$ at each point is transformed to $\Lambda\boldsymbol{r}^n$ with respect to the new axes, where Λ is an orthogonal matrix of order 3^n (Applequist 1983). It follows that $\mathbf{A}^{(n)}$ is transformed to $\Lambda\mathbf{A}^{(n)}$ with respect to the new axes, so that the transformed h_n is $\mathbf{A}^{(n)\mathrm{T}}\Lambda^{\mathrm{T}}\Lambda\boldsymbol{r}^n = \mathbf{A}^{(n)\mathrm{T}}\boldsymbol{r}^n$, an invariant under rotations. From this transformation property, $\mathbf{A}^{(n)}$ is a cartesian tensor of rank n (Jeffreys and Jeffreys 1962).

Comment. Since $\boldsymbol{r}^n$ is totally symmetric, we may rewrite (3.1) as

$$h_n(\boldsymbol{r}) = \mathbf{A}^{(n)}_{\mathrm{sym}} \cdot n \cdot \boldsymbol{r}^n \tag{3.2}$$

where $\mathbf{A}^{(n)}_{\mathrm{sym}}$ is the totally symmetric tensor defined by

$$A^{(n)}_{\mathrm{sym},\alpha_1\ldots\alpha_n} = \frac{1}{n!}\sum_{S\{\alpha\}} A^{(n)}_{\alpha_1\ldots\alpha_n}$$

where the sum is over all permutations of the symbols $\alpha_1\ldots\alpha_n$, regardless of their numerical values. Thus a homogeneous polynomial can always be expressed as a contraction of totally symmetric tensors. In what follows we will omit the subscript 'sym' in (3.2), as we will deal primarily with totally symmetric tensors.

3.2. *Tensor projections*

Let a direction in space be specified by the unit vector $\hat{\boldsymbol{r}} = \boldsymbol{r}/r$. Just as $\boldsymbol{a}\cdot\hat{\boldsymbol{r}}$ is the projection of the vector $\boldsymbol{a}$ along the direction $\hat{\boldsymbol{r}}$, $\mathbf{A}^{(n)} \cdot n \cdot \hat{\boldsymbol{r}}^n$ is the projection of the nth-rank tensor $\mathbf{A}^{(n)}$ along $\hat{\boldsymbol{r}}$. This may be seen by a simple example in which $\hat{\boldsymbol{r}}$ is directed along axis 3, i.e. $\hat{r}_\alpha = \delta_{3\alpha}$, the Kronecker delta. Then

$$\mathbf{A}^{(n)} \cdot n \cdot \hat{\boldsymbol{r}}^n = A^{(n)}_{\alpha_1\ldots\alpha_n}\delta_{3\alpha_1}\ldots\delta_{3\alpha_n} = A^{(n)}_{33\ldots3}$$

which is the component of $\mathbf{A}^{(n)}$ along axis 3. One obtains the same result for general $\hat{\boldsymbol{r}}$ by transforming $\mathbf{A}^{(n)}$ to a rotated coordinate system in which axis 3 lies along $\hat{\boldsymbol{r}}$. Thus we have a simple geometrical interpretation of the homogeneous polynomial of (3.1) as r^n times the projection of an nth-rank tensor.

3.3. *Linear independence*

The recognition of the linearly independent functions in a spherical harmonic expansion is essential in physical applications. The expansions used in the present cartesian tensor formalism employ functions that are not always linearly independent, so it is important to establish the linear independencies that do apply. The following lemma and its corollaries are cited to bring together certain independencies among homogeneous polynomials and distinguish them from a special case of surface spherical harmonics discussed in § 4.2.

Lemma. If $\mathbf{A}^{(n)}$ is a totally symmetric tensor, independent of $\boldsymbol{r}$, and $\mathbf{A}^{(n)} \cdot n \cdot \boldsymbol{r}^n \equiv 0$, then all components of $\mathbf{A}^{(n)}$ vanish.

Proof. From (2.2)

$$\mathbf{A}^{(n)} \cdot n \cdot \boldsymbol{r}^n = \sum_{n_1n_2n_3} g(n;n_1n_2n_3)A^{(n)}(n_1n_2n_3)x^{n_1}y^{n_2}z^{n_3} = 0.$$

It follows that $\mathbf{A}^{(n)} = 0$ because the terms $x^{n_1}y^{n_2}z^{n_3}$ are linearly independent.

Corollary I. If $\mathbf{A}^{(n)}$ is a totally symmetric tensor, independent of $\boldsymbol{r}$, and $\mathbf{A}^{(n)} \cdot n \cdot \hat{\boldsymbol{r}}^n \equiv 0$, then all components of $\mathbf{A}^{(n)}$ vanish.

Comment. The corollary means that a totally symmetric nth-rank tensor vanishes if its projection in all directions vanishes.

Corollary II. If $\mathbf{A}^{(n)}$ is a totally symmetric tensor, independent of $\boldsymbol{r}$, for all n and

$$\sum_{n=0}^{\infty} \mathbf{A}^{(n)} \cdot n \cdot \boldsymbol{r}^n \equiv 0$$

then $\mathbf{A}^{(n)} = 0$ for all n.

Proof. The terms of the sum are homogeneous polynomials of different degrees and are, therefore, linearly independent. Hence $\mathbf{A}^{(n)} \cdot n \cdot \boldsymbol{r}^n \equiv 0$ for all n. The corollary follows from the above lemma.

3.4. Gradient theorem

The following gradient theorem is fundamental for homogeneous polynomials and is useful in electrostatic problems. We employ the gradient operator $\nabla \equiv \partial/\partial \boldsymbol{r}$.

Theorem. If $h_n(\boldsymbol{r}) = \mathbf{A}^{(n)} \cdot n \cdot \boldsymbol{r}^n$ and $\mathbf{A}^{(n)}$ is a totally symmetric tensor, independent of $\boldsymbol{r}$, then

$$\nabla^k h_n(\boldsymbol{r}) = \frac{n!}{(n-k)!} \mathbf{A}^{(n)} \cdot (n-k) \cdot \boldsymbol{r}^{n-k} \tag{3.3}$$

for $k = 0, 1, \ldots, n$.

Proof. We have

$$\begin{aligned} \nabla_\beta h_n &= \nabla_\beta A^{(n)}_{\alpha_1 \ldots \alpha_n} r_{\alpha_1} \ldots r_{\alpha_n} \\ &= A^{(n)}_{\alpha_1 \ldots \alpha_n} (\delta_{\alpha_1 \beta} r_{\alpha_2} \ldots r_{\alpha_n} + \ldots + r_{\alpha_1} \ldots r_{\alpha_{n-1}} \delta_{\alpha_n \beta}) \\ &= n \mathbf{A}^{(n)} \cdot (n-1) \cdot \boldsymbol{r}^{n-1} \end{aligned}$$

which proves the theorem for $k = 1$. Assuming (3.3) to be true for the kth gradient, one finds by the same differentiation process that it holds for the $(k+1)$th gradient. The theorem follows by induction.

The theorem shows that each component of the kth-rank tensor $\nabla^k h_n(\boldsymbol{r})$ is a homogeneous polynomial of degree $n - k$.

3.5. Generalised Euler theorem

An immediate consequence of the gradient theorem is the following generalised Euler theorem for homogeneous polynomials. The Euler theorem is usually stated only for $k = 1$ (see, for example, Chaundy 1935).

Theorem. If $h_n(\boldsymbol{r})$ is a homogeneous polynomial of degree n ($n \geq 0$), then

$$\boldsymbol{r}^k \cdot k \cdot \nabla^k h_n(\boldsymbol{r}) = \frac{n!}{(n-k)!} h_n(\boldsymbol{r}) \tag{3.4}$$

for $k = 0, 1, \ldots, n$.

Proof. Equation (3.4) follows from (3.3) by contracting $\boldsymbol{r}^k$ with both sides of the latter.

4. Spherical harmonics as tensor contractions

Hobson (1931) defines *ordinary* spherical harmonics of degree n, a non-negative integer, as spherical harmonics which are polynomials of degree n in x, y, z, together with the corresponding harmonics of negative degree $-n-1$, obtained by multiplication of the former by r^{-2n-1}. This is the class of spherical harmonics with which physics is primarily concerned, and we will not deal with the more general class (Hobson 1931, p163, p178).

4.1. Tensor contraction theorem

We seek a criterion for those homogeneous polynomials which satisfy the Laplace equation. This is supplied by the following theorem. The theorem paraphrases, in tensor notation, a relation among polynomial coefficients that has been demonstrated for specific cases (Whittaker and Watson 1927, MacRobert 1947, p134). The theorem is central to the formalism of this paper, and a proof is in order.

Theorem. If $\mathbf{A}^{(n)}$ is a totally symmetric tensor, independent of $\boldsymbol{r}$, and $f_n(\boldsymbol{r}) \equiv \mathbf{A}^{(n)} \cdot n \cdot \boldsymbol{r}^n$, then f_n is a solid spherical harmonic of degree n if and only if $\mathbf{A}^{(n)}$ is totally traceless.

Proof. Since f_n is homogeneous of degree n (§ 3.1), it remains to show that the Laplace equation is satisfied. For $n \geq 2$, (3.3) gives

$$\nabla_\nu \nabla_\nu f_n(\boldsymbol{r}) = n(n-1) A^{(n)}_{\nu\nu\alpha_3\ldots\alpha_n} r_{\alpha_3} \ldots r_{\alpha_n} = 0$$

the last equality being true for all $\boldsymbol{r}$ if and only if $A^{(n)}_{\nu\nu\alpha_3\ldots\alpha_n}$ vanishes; i.e. the Laplace equation is satisfied if and only if $\mathbf{A}^{(n)}$ is totally traceless. For $n = 0$ or 1 the theorem is trivial.

From the Kelvin theorem (MacRobert 1947, p74) we have the following corollary.

Corollary. If $\mathbf{A}^{(n)}$ is a totally symmetric tensor, independent of $\boldsymbol{r}$, then $r^{-2n-1}\mathbf{A}^{(n)} \cdot n \cdot \boldsymbol{r}^n$ is a solid spherical harmonic of degree $-n-1$ if and only if $\mathbf{A}^{(n)}$ is totally traceless.

From the definition of a surface spherical harmonic as a solid spherical harmonic evaluated at $r = 1$ we have another corollary.

Corollary. If $\mathbf{A}^{(n)}$ is a totally symmetric tensor, independent of $\boldsymbol{r}$, then $\mathbf{A}^{(n)} \cdot n \cdot \hat{\boldsymbol{r}}^n$ is a surface spherical harmonic of degree n if and only if $\mathbf{A}^{(n)}$ is totally traceless.

4.2. Linear independence of surface spherical harmonics

We return to the question of linear independence raised in § 3.3, where the independence of terms in a homogeneous polynomial led to a criterion for the vanishing of a symmetric tensor $\mathbf{A}^{(n)}$. The following theorem broadens the criterion to a vanishing sum of tensor projections, but only under the condition that the tensors be traceless as well as symmetric.

Theorem. If $\mathbf{A}^{(n)}$ is a totally symmetric and traceless tensor, independent of $\boldsymbol{r}$, for all n and

$$\sum_{n=0}^{\infty} \mathbf{A}^{(n)} \cdot n \cdot \hat{\boldsymbol{r}}^n \equiv 0 \tag{4.1}$$

then $\mathbf{A}^{(n)} = 0$ for all n.

Proof. The summand of (4.1) is a surface spherical harmonic of degree n. Surface spherical harmonics of different degrees are mutually orthogonal (Hobson 1931, p144) and, hence, linearly independent. Thus $\mathbf{A}^{(n)} \cdot n \cdot \hat{\boldsymbol{r}}^n = 0$ for all n. The theorem follows by corollary I of § 3.3.

Comment. The theorem does not imply that all components of $\hat{\boldsymbol{r}}^n$ for all n are linearly independent, and in fact one can find sets of coefficients, not all zero, such that the sum of terms vanishes; e.g. $\hat{x}^2 + \hat{y}^2 + \hat{z}^2 - 1 \equiv 0$. However, such coefficients do not constitute traceless tensors, and the theorem would not apply if $\mathbf{A}^{(n)}$ were not both traceless and symmetric. On the other hand, the restriction to traceless tensors does not apply to the corresponding case of general homogeneous polynomials, as seen in corollary II of § 3.3.

5. The detracer operator

The detracer $\mathscr{T}_n$ is an operator which acts on a totally symmetric tensor $\mathbf{A}^{(n)}$ so that $\mathscr{T}_n\mathbf{A}^{(n)}$ is a totally symmetric and traceless tensor of rank n. This operator plays a major role in generating cartesian tensor forms for spherical harmonic functions. The operator and some of its properties have been employed previously (Applequist 1984, 1985). A fuller development is supplied here.

5.1. The detracer theorem

We define $\mathscr{T}_n$ by

$$\mathscr{T}_n A^{(n)}_{\alpha_1 \ldots \alpha_n} = \sum_{m=0}^{[n/2]} (-1)^m (2n-2m-1)!! \sum_{T\{\alpha\}} \delta_{\alpha_1\alpha_2} \ldots \delta_{\alpha_{2m-1}\alpha_{2m}} A^{(n:m)}_{\alpha_{2m+1}\ldots\alpha_n} \tag{5.1}$$

where $[n/2]$ denotes the largest integer not exceeding $n/2$ and the sum over $T\{\alpha\}$ is the sum over all permutations of the symbols $\alpha_1 \ldots \alpha_n$ which give distinct terms. The odd factorial $(2k-1)!!$ is defined as $1 \times 3 \times 5 \times \ldots \times (2k-1)$, with $(-1)!! = 1$.

Theorem. If $\mathbf{A}^{(n)}$ is a totally symmetric tensor of rank n, and $\mathbf{B}^{(n)} = \mathscr{T}_n\mathbf{A}^{(n)}$, then $\mathbf{B}^{(n)}$ is a totally symmetric and traceless tensor of rank n.

Proof. The total symmetry of $\mathbf{B}^{(n)}$ is ensured by the summation over distinct permutations of indices in (5.1). It remains to show that $\mathbf{B}^{(n:1)} = 0$. When we take the trace in indices $\alpha_1\alpha_2$, (5.1) gives

$$B^{(n:1)}_{\alpha_3\ldots\alpha_n} = \sum_{k=1}^{[n/2]} C_{n,k} \sum_{T\{\alpha\}} \delta_{\alpha_3\alpha_4} \ldots \delta_{\alpha_{2k-1}\alpha_{2k}} A^{(n:k)}_{\alpha_{2k+1}\ldots\alpha_n} \tag{5.2}$$

where the $C_{n,k}$ are coefficients which will be shown to vanish. Through the permutations of indices, the terms in (5.2) arise in the following four ways.

(i) α_1 and α_2 occur in the factor $\delta_{\alpha_1\alpha_2}$, whose trace is 3. Terms in (5.2) arise from terms in (5.1) with $m = k$. The contribution to $C_{n,k}$ is thus $3(-1)^k(2n-2k-1)!!$.

(ii) α_1 and α_2 occur in separate factors $\delta_{\alpha_1\alpha_p}$ and $\delta_{\alpha_2\alpha_q}$, giving a factor $\delta_{\alpha_p\alpha_q}$ in the trace. Terms in (5.2) arise from terms in (5.1) with $m = k$. The factor $\delta_{\alpha_p\alpha_q}$ in (5.2) may arise from either $\delta_{\alpha_1\alpha_p}\delta_{\alpha_2\alpha_q}$ or $\delta_{\alpha_1\alpha_q}\delta_{\alpha_2\alpha_p}$ in (5.1), and any of the $k-1$ δ factors in (5.2) may arise in this way. The contribution to $C_{n,k}$ is therefore $2(k-1)(-1)^k(2n-2k-1)!!$.

(iii) α_1 and α_2 occur in the factor $\mathbf{A}^{(n:m)}$ in (5.1). On taking the trace, a term in $\mathbf{A}^{(n:k)}$ arises in (5.2) with $k = m+1$. The contribution to $C_{n,k}$ is thus $(-1)^{k-1}(2n-2k+1)!!$.

(iv) α_1 occurs in a factor of $\delta_{\alpha_1\alpha_p}$, and α_2 occurs in the factor $\mathbf{A}^{(n:m)}$, giving rise to a term in $\mathbf{A}^{(n:k)}$ with $k = m$ and α_p substituted for α_2. The same term arises from that in which α_1 and α_2 are interchanged, and α_p can be any of the $n-2k$ indices of $\mathbf{A}^{(n:k)}$. Hence, the contribution to $C_{n,k}$ is $2(n-2k)(-1)^k(2n-2k-1)!!$.

Thus we have

$$\begin{aligned} C_{n,k} &= (-1)^k(2n-2k-1)!![3+2(k-1)-(2n-2k+1)+2(n-2k)] \\ &= 0 \end{aligned}$$

which completes the proof.

Corollary. If $\mathbf{B}^{(n)}$ is a totally symmetric and traceless tensor of rank n, then

$$\mathscr{T}_n\mathbf{B}^{(n)} = (2n-1)!!\mathbf{B}^{(n)}. \tag{5.3}$$

Proof. Since all traces vanish, the only remaining term in (5.1) is that for $m = 0$. The result is (5.3).

Note. It may be noted that the detracer is a projection operator in that it projects out of a general symmetric tensor of rank n that irreducible part which transforms as a tensor of rank n (McWeeny 1963, Gray and Gubbins 1984, p490). However, $\mathscr{T}_n$ lacks the property of idempotency usually associated with a projection operator; i.e. $\mathscr{T}_n\mathscr{T}_n \neq \mathscr{T}_n$. We may define another detracer $\mathscr{D}_n = [(2n-1)!!]^{-1}\mathscr{T}_n$, which, by (5.3) satisfies $\mathscr{D}_n\mathscr{D}_n = \mathscr{D}_n$, and is therefore a true projection operator. The operator $\mathscr{T}_n$ is more firmly associated with the theory of multipole moments and the gradients of $1/r$ (Applequist 1984), and is therefore retained in the present work. Should $\mathscr{D}_n$ prove more desirable in any application, its substitution for $\mathscr{T}_n$ is a simple matter.

5.2. The detracer exchange theorem

The following theorem and its corollary make possible some important transformations of spherical harmonic expressions.

Theorem. If $\mathbf{A}^{(n)}$ and $\mathbf{B}^{(n)}$ are totally symmetric tensors of rank n, then

$$\mathbf{A}^{(n)} \cdot n \cdot \mathscr{T}_n\mathbf{B}^{(n)} = \mathbf{B}^{(n)} \cdot n \cdot \mathscr{T}_n\mathbf{A}^{(n)}. \tag{5.4}$$

Proof. The theorem follows by expanding each side of (5.4) according to (5.1).

Corollary. If $\mathbf{A}^{(n)}$ and $\mathbf{B}^{(n)}$ are totally symmetric tensors of rank n, then

$$\mathscr{T}_n\mathbf{A}^{(n)} \cdot n \cdot \mathscr{T}_n\mathbf{B}^{(n)} = (2n-1)!!\mathbf{A}^{(n)} \cdot n \cdot \mathscr{T}_n\mathbf{B}^{(n)}. \tag{5.5}$$

Proof. From (5.4) we have

$$\mathscr{T}_n\mathbf{A}^{(n)} \cdot n \cdot \mathscr{T}_n\mathbf{B}^{(n)} = \mathbf{A}^{(n)} \cdot n \cdot \mathscr{T}_n\mathscr{T}_n\mathbf{B}^{(n)}$$

which becomes (5.5) by use of (5.3).

5.3. *The detracer for compressed tensors*

It is often more convenient to work with compressed tensors (Applequist 1983) than with the complete tensors of (5.1). We obtain here the form of $\mathscr{T}_n$ appropriate to such tensors. In (5.1) the non-vanishing terms are those containing traces of the form $A^{(n:m)}(n_1-2m_1, n_2-2m_2, n_3-2m_3)$, where $2m_i \le n_i$, $n_1+n_2+n_3 = n$, and $m_1+m_2+m_3 = m$. The number of times this term occurs in the sum over $T\{\alpha\}$ is the number of ways m_1 distinct pairs of symbols $\alpha_i\alpha_j$ can be selected from those symbols among $\alpha_1 \ldots \alpha_n$ which take the value 1, times the corresponding numbers for m_2 and m_3 pairs. The number of ways of selecting m distinct pairs of objects from n distinct objects is

$$\begin{bmatrix} n \\ m \end{bmatrix} = \frac{n!}{2^m m!(n-2m)!}.$$

Thus (5.1) becomes

$$\mathscr{T}_n\mathbf{A}^{(n)} = \sum_{m_1=0}^{[n_1/2]} \sum_{m_2=0}^{[n_2/2]} \sum_{m_3=0}^{[n_3/2]} (-1)^m(2n-2m-1)!! \times \begin{bmatrix} n_1 \\ m_1 \end{bmatrix} \begin{bmatrix} n_2 \\ m_2 \end{bmatrix} \begin{bmatrix} n_3 \\ m_3 \end{bmatrix} A^{(n:m)}(n_1-2m_1, n_2-2m_2, n_3-2m_3). \tag{5.6}$$

With (2.4) this provides the means of constructing the traceless form of a compressed tensor.

5.4. *The detracer in tensor form*

The detracing operation of (5.1) is a linear combination of components of the tensor $\mathbf{A}^{(n)}$, and is expressible as a tensor contraction. It will help to complete the discussion of $\mathscr{T}_n$ to give the tensor form of this operator. Let $\mathbf{A}^{(n)}$ be a totally symmetric tensor, and let $\mathbf{B}^{(n)} = \mathscr{T}_n\mathbf{A}^{(n)}$. Then we require a tensor of subdivided rank $\mathscr{T}^{(n,n)}$ (Applequist 1983) such that

$$B^{(n)}_{\beta_1\ldots\beta_n} = \mathscr{T}^{(n,n)}_{\beta_1\ldots\beta_n,\alpha_1\ldots\alpha_n} A^{(n)}_{\alpha_1\ldots\alpha_n}. \tag{5.7}$$

From (2.3) and (5.1) it can be seen that

$$\mathscr{T}^{(n,n)}_{\beta_1\ldots\beta_n,\alpha_1\ldots\alpha_n} = \sum_{m=0}^{[n/2]} (-1)^m(2n-2m-1)!! \times \sum_{T\{\alpha\beta\}} \delta_{\alpha_1\alpha_2}\ldots\delta_{\alpha_{2m-1}\alpha_{2m}}\delta_{\beta_1\beta_2}\ldots\delta_{\beta_{2m-1}\beta_{2m}}\delta_{\alpha_{2m+1}\beta_{2m+1}}\ldots\delta_{\alpha_n\beta_n} \tag{5.8}$$

where the sum over $T\{\alpha\beta\}$ is the sum over all identical permutations of the sets $\alpha_1 \ldots \alpha_n$ and $\beta_1 \ldots \beta_n$ giving distinct terms. For example, (5.8) gives for $n = 3$

$$\mathscr{T}^{(3,3)}_{\beta_1\beta_2\beta_3,\alpha_1\alpha_2\alpha_3} = 15\delta_{\alpha_1\beta_1}\delta_{\alpha_2\beta_2}\delta_{\alpha_3\beta_3} - 3(\delta_{\alpha_1\alpha_2}\delta_{\beta_1\beta_2}\delta_{\alpha_3\beta_3} + \delta_{\alpha_1\alpha_3}\delta_{\beta_1\beta_3}\delta_{\alpha_2\beta_2} + \delta_{\alpha_2\alpha_3}\delta_{\beta_2\beta_3}\delta_{\alpha_1\beta_1})$$

so that, from (5.7),

$$B^{(3)}_{\beta_1\beta_2\beta_3} = 15A^{(3)}_{\beta_1\beta_2\beta_3} - 3(A^{(3)}_{\nu\nu\beta_3}\delta_{\beta_1\beta_2} + A^{(3)}_{\nu\nu\beta_2}\delta_{\beta_1\beta_3} + A^{(3)}_{\nu\nu\beta_1}\delta_{\beta_2\beta_3})$$

in agreement with the result from direct application of (5.1) (Applequist 1984). It can be shown that $\mathscr{T}^{(n,n)}$ is an isotropic tensor of rank $2n$ from its transformation under rotation of coordinate axes and that the tensor is totally symmetric and traceless within each index set $\alpha_1 \ldots \alpha_n$ and $\beta_1 \ldots \beta_n$.

6. Gradients of r^{-1} as spherical harmonics

Maxwell first derived a general expression for a solid spherical harmonic of degree $-n-1$ as the nth-order gradient of r^{-1} with respect to a set of n arbitrary axes (Hobson 1931, p131). When all of the axes coincide with cartesian axes, his formula for the gradient reduces to

$$\nabla^n r^{-1} = (-1)^n r^{-2n-1} \mathscr{T}_n \boldsymbol{r}^n. \tag{6.1}$$

This relation has been given previously (Applequist 1984) with the observation that it is equivalent to a relation obtained by Burgos and Bonadeo (1981) by another route. Equation (6.1) leads to two important conclusions: (i) the components of the tensor $\mathscr{T}_n \boldsymbol{r}^n$ are solid spherical harmonics of degree n, and (ii) the components of the tensor $\mathscr{T}_n \hat{\boldsymbol{r}}^n$ are surface spherical harmonics of degree n. An example is given in (1.1), where $f = \mathscr{T}_2 x^2$. These functions will be referred to here as 'cartesian basis' spherical harmonics because they are special forms of Maxwell's spherical harmonics based on the cartesian axes. The name is appropriate for the following reason as well: a general solid spherical harmonic $\mathbf{A}^{(n)} \cdot n \cdot \boldsymbol{r}^n$ (with traceless $\mathbf{A}^{(n)}$) can be expressed in the form

$$\mathbf{A}^{(n)} \cdot n \cdot \boldsymbol{r}^n = \frac{1}{(2n-1)!!} \mathbf{A}^{(n)} \cdot n \cdot \mathscr{T}_n \boldsymbol{r}^n$$

by applying (5.3) and (5.5). Thus the general harmonic is expressed as a linear combination of the cartesian basis harmonics using coefficients that are the same, aside from a constant factor, as those appearing in the linear combination of $\boldsymbol{r}^n$ functions.

It is worth noting that the components of $\mathscr{T}_n \boldsymbol{r}^n$ themselves conform to the general tensor contraction expression of § 4.1, since $\mathscr{T}_n \boldsymbol{r}^n = \mathscr{T}^{(n,n)} \cdot n \cdot \boldsymbol{r}^n$, by (5.7).

Equation (6.1) serves as a means of simplifying expressions involving the gradients, using the properties of the detracer (Applequist 1985). The form of $\mathscr{T}_n \boldsymbol{r}^n$ obtained from (5.1) is usually suitable when needed in this connection. An alternative form which is useful for some analytical purposes and is especially efficient for numerical calculations may be obtained from the compressed tensor formalism. Since

$$r^{2m} = \sum_{k_1 k_2 k_3} g(m; k_1 k_2 k_3) x^{2k_1} y^{2k_2} z^{2k_3}$$

we have, from (2.4) and (5.6),

$$\mathscr{T}_n x^{n_1} y^{n_2} z^{n_3} = \sum_{m_1=0}^{[n_1/2]} \sum_{m_2=0}^{[n_2/2]} \sum_{m_3=0}^{[n_3/2]} (-1)^m (2n-2m-1)!! \times \begin{bmatrix} n_1 \\ m_1 \end{bmatrix} \begin{bmatrix} n_2 \\ m_2 \end{bmatrix} \begin{bmatrix} n_3 \\ m_3 \end{bmatrix} r^{2m} x^{n_1-2m_1} y^{n_2-2m_2} z^{n_3-2m_3}. \tag{6.2}$$

Here $\mathscr{T}_n x^{n_1} y^{n_2} z^{n_3}$ denotes a component of $\mathscr{T}_n \boldsymbol{r}^n$ specified by indices $n_1 n_2 n_3$. (Strictly speaking, $\mathscr{T}_n$ operates only on the full set of components of $\boldsymbol{r}^n$ and not on an individual component.) Equations (6.1) and (6.2) together are equivalent to gradient formulae derived by other routes by Burgos and Bonadeo (1981) and by Cipriani and Silvi (1982).

7. Legendre polynomials

7.1. Cartesian tensor form for Legendre polynomials

The Legendre polynomial $P_n(\cos\theta)$ of degree n is a surface spherical harmonic which is widely used in harmonic expansions because of its natural origin in potential functions and its convenient properties of recurrence, differentiation, and integration (Hobson 1931, MacRobert 1947). The connection between the Legendre polynomials and the cartesian basis spherical harmonics, established in this section, provides a basis for transforming expansions from Legendre polynomial form to cartesian tensor form, and vice versa.

Theorem. Given vectors $\boldsymbol{r}, \boldsymbol{s}$ and the associated unit vectors $\hat{\boldsymbol{r}}, \hat{\boldsymbol{s}}$

$$P_n(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{s}}) = \frac{1}{n!} \hat{\boldsymbol{s}}^n \cdot n \cdot \mathscr{T}_n \hat{\boldsymbol{r}}^n = \frac{1}{n!} \hat{\boldsymbol{r}}^n \cdot n \cdot \mathscr{T}_n \hat{\boldsymbol{s}}^n \tag{7.1}$$

for $n = 0, 1, 2, \ldots$.

Proof. Let $R = |\boldsymbol{r} - \boldsymbol{s}|$. Then $\partial^n R^{-1}/\partial \boldsymbol{s}^n = (-1)^n \partial^n R^{-1}/\partial \boldsymbol{r}^n$, and the Taylor expansion for R^{-1} about $\boldsymbol{s} = \boldsymbol{0}$ becomes

$$R^{-1} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \boldsymbol{s}^n \cdot n \cdot \nabla^n r^{-1}.$$

With (6.1) this becomes

$$R^{-1} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{s^n}{r^{n+1}} \right) \hat{\boldsymbol{s}}^n \cdot n \cdot \mathscr{T}_n \hat{\boldsymbol{r}}^n$$

which converges for $s < r$. But the coefficient of s^n/r^{n+1} in this expansion is, by definition, $P_n(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{s}})$ (MacRobert 1947, p73). Hence the first equality in (7.1) is proved. The second equality follows either from (5.4) or from the fact that the equation must hold when $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{s}}$ are interchanged.

Corollary I. For $\hat{x} = x/r$,

$$P_n(\hat{x}) = \frac{1}{n!}\mathscr{T}_n\hat{x}^n. \tag{7.2}$$

Proof. The corollary follows from (7.1) by letting $\hat{s}$ be directed along the positive x axis.

Corollary II. Given unit vectors $\hat{r}$ and $\hat{s}$,

$$P_n(\hat{r}\cdot\hat{s}) = \frac{2^n}{(2n)!}\mathscr{T}_n\hat{r}^n \cdot n \cdot \mathscr{T}_n\hat{s}^n \tag{7.3}$$

for $n = 0, 1, 2, \ldots$.

Proof. The corollary follows from (5.5) and (7.1), using $(2n-1)!! = (2n)!/2^n n!$.

Comment. Equation (7.3) is an 'addition theorem' analogous to the better known relation (Edmonds 1974, p63)

$$P_n(\hat{r}\cdot\hat{s}) = \sum_{m=-n}^{n} \frac{(n-m)!}{(n+m)!} Y_n^m(\theta,\phi) Y_n^{m*}(\theta',\phi') \tag{7.4}$$

where

$$Y_n^m(\theta,\phi) = P_n^m(\cos\theta)\mathrm{e}^{\mathrm{i}m\phi} \tag{7.5}$$

and (θ,ϕ) are the spherical angles defining $\hat{r}$ and (θ',ϕ') are those defining $\hat{s}$. The right-hand sides of both (7.3) and (7.4) are sums of products of surface spherical harmonics evaluated at $\hat{r}$ and $\hat{s}$. An important distinction is that the sum in (7.4) includes only $2n+1$ products, while that in (7.3) includes $(n+1)(n+2)/2$ distinct products.

Corollary III. Given unit vector $\hat{r}$,

$$\mathscr{T}_n\hat{r}^n \cdot n \cdot \mathscr{T}_n\hat{r}^n = (2n)!/2^n \tag{7.6}$$

for $n = 0, 1, 2, \ldots$.

Proof. The corollary follows from (7.3), setting $\hat{s} = \hat{r}$, and using $P_n(1) = 1$ for $n = 0, 1, 2, \ldots$.

The left-hand side of (7.6) is the sum of squares of a set of surface spherical harmonics of degree n evaluated at $\hat{r}$. The corollary says that this sum is independent of direction in space. A well-known analogy is the Unsöld theorem (Slater 1968),

$$\sum_{m=-n}^{n} \frac{(n-m)!}{(n+m)!} Y_n^m(\theta,\phi) Y_n^{m*}(\theta,\phi) = 1.$$

Note. The real and imaginary parts of Y_n^m are each surface spherical harmonics known collectively as 'tesseral and sectoral surface harmonics of the first kind' (Hobson 1931, p91; Abramowitz and Stegun 1965). The notation of (7.5) follows Böttcher (1952, p90), and the Y_n^m so defined are referred to here simply as tesseral harmonics. The normalised versions of these functions, commonly denoted Y_{nm}, appear widely in quantum mechanical applications and in the theory of spherical tensors (Edmonds 1974, p24, Gray and Gubbins 1984, p442).

7.2. Derivative theorem for Legendre polynomials

We give here a further theorem that is useful in transforming a spherical harmonic expansion from a tensor contraction form to a Legendre polynomial form which is useful for numerical computations. It will be noted that both forms are based on cartesian tensors.

Theorem. Given vectors $\boldsymbol{r}$ and $\boldsymbol{s}$,

$$\boldsymbol{s}^{n-k} \cdot (n-k) \cdot \mathcal{T}_n \boldsymbol{r}^n = (n-k)!\, r^n \frac{\partial^k}{\partial \boldsymbol{s}^k} s^n P_n(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{s}}) \tag{7.7}$$

for $k = 0, 1, 2, \ldots, n$.

Proof. The theorem follows from (3.3), letting $\mathbf{A}^n = \mathcal{T}_n \boldsymbol{r}^n$ and applying (7.1).

Lemma. Given a function $f(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{s}})$ whose derivative $f'(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{s}})$ with respect to the argument exists,

$$\frac{\partial}{\partial \boldsymbol{s}} f(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{s}}) = s^{-1} \hat{\boldsymbol{r}} \cdot (\mathbf{I} - \hat{\boldsymbol{s}}\hat{\boldsymbol{s}}) f'(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{s}}) \tag{7.8}$$

where $\mathbf{I}$ is the second rank identity tensor.

Proof. Using component notation,

$$\begin{aligned} \frac{\partial f}{\partial s_\alpha} &= f' \frac{\partial}{\partial s_\alpha} \hat{r}_\nu \hat{s}_\nu = f' \hat{r}_\nu \frac{\partial}{\partial s_\alpha} (s_\nu / s) \\ &= f' \hat{r}_\nu (\delta_{\alpha\nu}/s - s_\nu s_\alpha / s^3) \\ &= f' s^{-1} \hat{r}_\nu (\delta_{\alpha\nu} - \hat{s}_\nu \hat{s}_\alpha) \quad (7.8) \end{aligned}$$

The following are examples of (7.7) for $k = 1, 2, n$, respectively. The first two are derived using (7.8). The expressions are obtained in terms of unit vectors by dividing through by $r^n s^{n-k}$ after performing the differentiations:

$$\hat{\boldsymbol{s}}^{n-1} \cdot (n-1) \cdot \mathcal{T}_n \hat{\boldsymbol{r}}^n = (n-1)!\,[\hat{\boldsymbol{r}} P_n'(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{s}}) - \hat{\boldsymbol{s}} P_{n-1}'(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{s}})] \tag{7.9}$$

$$\begin{aligned} &\hat{\boldsymbol{s}}^{n-2} \cdot (n-2) \cdot \mathcal{T}_n \hat{\boldsymbol{r}}^n \\ &\quad = (n-2)!\,[\hat{\boldsymbol{r}}\hat{\boldsymbol{r}} P_n''(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{s}}) + \hat{\boldsymbol{s}}\hat{\boldsymbol{s}} P_{n-2}''(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{s}}) - (\hat{\boldsymbol{r}}\hat{\boldsymbol{s}} + \hat{\boldsymbol{s}}\hat{\boldsymbol{r}}) P_{n-1}''(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{s}}) - I P_{n-1}'(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{s}})] \end{aligned} \tag{7.10}$$

$$\mathcal{T}_n \hat{\boldsymbol{r}}^n = \frac{\partial^n}{\partial \boldsymbol{s}^n} s^n P_n(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{s}}). \tag{7.11}$$

Equations (7.9) and (7.10) will reappear in certain multipole potentials in § 9. Equation (7.11) is an additional identity relating the surface spherical harmonics $\mathcal{T}_n \hat{\boldsymbol{r}}^n$ and $P_n(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{s}})$, complementary to (7.1).

8. Cartesian basis spherical harmonics

In § 6 we found that the components of the tensor $\mathcal{T}_n \hat{\boldsymbol{r}}^n$ are surface spherical harmonics, and in § 7.1 we saw that these functions obey an addition theorem and an 'Unsöld' theorem analogous to those for the tesseral harmonics $Y_n^m(\theta, \phi)$. Such properties suggest that the cartesian basis surface spherical harmonics might find wider use in roles normally filled by $Y_n^m(\theta, \phi)$. It seems worthwhile, therefore, to develop here some of the further general properties of $\mathcal{T}_n \hat{\boldsymbol{r}}^n$ for future reference. Aside from certain relations in § 8.1, the results in this section are not needed for the electrostatic problems that follow.

8.1. Relations among gradients and harmonics of successive degrees

This subsection deals primarily with the solid spherical harmonics $\mathscr{T}_n\boldsymbol{r}^n$, which are likely to be of greater significance than the surface harmonics when dealing with the three-dimensional gradients. The selection of identities here is limited to a few which seem particularly novel and significant. Others can be derived by combinations of those given. The known recurrence relations among the Legendre polynomials (Hobson 1931, p32) lead to further identities in $\mathscr{T}_n\hat{\boldsymbol{r}}^n$ by way of (7.1), none of which are included here. The gradient operator $\nabla \equiv \partial/\partial\boldsymbol{r}$ is used throughout.

Theorem.

$$\boldsymbol{r}\cdot\mathscr{T}_{n+1}\boldsymbol{r}^{n+1} = (n+1)r^2\mathscr{T}_n\boldsymbol{r}^n. \tag{8.1}$$

Proof. Since $\nabla^n r^{-1}$ is homogeneous of degree $-n-1$, Euler's theorem gives

$$\boldsymbol{r}\cdot\nabla^{n+1}r^{-1} = -(n+1)\nabla^n r^{-1}.$$

The result (8.1) then follows by using (6.1).

Theorem.

$$\boldsymbol{r}^k\cdot k\cdot\nabla^k\mathscr{T}_n\boldsymbol{r}^n = \frac{n!}{(n-k)!}\mathscr{T}_n\boldsymbol{r}^n \qquad k=0,1,\ldots,n. \tag{8.2}$$

Proof. The theorem follows from (3.4) and the fact that the components of $\mathscr{T}_n\boldsymbol{r}^n$ are homogeneous of degree n.

Theorem.

$$(\boldsymbol{r}\cdot\nabla)^k\mathscr{T}_n\boldsymbol{r}^n = n^k\mathscr{T}_n\boldsymbol{r}^n \qquad k=0,1,\ldots,\infty. \tag{8.3}$$

Proof. Euler's theorem gives

$$\boldsymbol{r}\cdot\nabla\mathscr{T}_n\boldsymbol{r}^n = n\mathscr{T}_n\boldsymbol{r}^n.$$

Equation (8.3) is obtained by applying the operator $\boldsymbol{r}\cdot\nabla$ to the last equation $k-1$ times.

Comment. The operator $(\boldsymbol{r}\cdot\nabla)^k$ in (8.3) is distinct from the operator $\boldsymbol{r}^k\cdot k\cdot\nabla^k$ in (8.2) in that each factor $\boldsymbol{r}\cdot\nabla$ operates on both the $\boldsymbol{r}$ and ∇ parts of each factor following it in the former.

Theorem.

$$r^2\nabla\mathscr{T}_n\boldsymbol{r}^n = (2n+1)\boldsymbol{r}\mathscr{T}_n\boldsymbol{r}^n - \mathscr{T}_{n+1}\boldsymbol{r}^{n+1}. \tag{8.4}$$

Proof. Taking the gradient of both sides of (6.1), we have

$$\begin{aligned}\nabla^{n+1}r^{-1} &= (-1)^n[-(2n+1)r^{-2n-3}\boldsymbol{r}\mathscr{T}_n\boldsymbol{r}^n + r^{-2n-1}\nabla\mathscr{T}_n\boldsymbol{r}^n]\\ &= (-1)^{n+1}r^{-2n-3}\mathscr{T}_{n+1}\boldsymbol{r}^{n+1}.\end{aligned}$$

Equation (8.4) follows by rearrangement. Note that ∇ and $\boldsymbol{r}$ appearing as prefactors in (8.4) must have the same component indices, since they belong to tensors which are not totally symmetric.

Corollary.

$$r\nabla\mathscr{T}_n\hat{\boldsymbol{r}}^n = (n+1)\hat{\boldsymbol{r}}\mathscr{T}_n\hat{\boldsymbol{r}}^n - \mathscr{T}_{n+1}\hat{\boldsymbol{r}}^{n+1}. \tag{8.5}$$

Proof. Equation (8.5) follows from (8.4) by inserting the relation

$$\nabla\mathscr{T}_n\boldsymbol{r}^n = \nabla r^n\mathscr{T}_n\hat{\boldsymbol{r}}^n = nr^{n-2}\boldsymbol{r}\mathscr{T}_n\hat{\boldsymbol{r}}^n + r^n\nabla\mathscr{T}_n\hat{\boldsymbol{r}}^n.$$

8.2. Linearly independent subsets of $\mathscr{T}_n\hat{r}^n$

The number of linearly independent surface spherical harmonics of degree n is $2n+1$. However, $\mathscr{T}_n\hat{r}^n$, in the form of a compressed tensor $\mathscr{T}_n\hat{x}^{n_1}\hat{y}^{n_2}\hat{z}^{n_3}$, has $(n+1)(n+2)/2$ components with different indices $n_1n_2n_3$. These are not all independent owing to the fact that the tensor is totally traceless. The 1-fold trace, being a tensor of rank $n-2$, contains $n(n-1)/2$ components, each of which, set equal to zero, gives a linear relation among three components of $\mathscr{T}_n\hat{r}^n$. Hence, the number of independent components of this tensor is $(n+1)(n+2)/2 - n(n-1)/2 = 2n+1$, as required. The following theorem provides a means of choosing a subset of linearly independent components.

Theorem. The components of $\mathscr{T}_n\hat{x}^{n_1}\hat{y}^{n_2}\hat{z}^{n_3}$ in which $n_3 = 0$ or 1 constitute a linearly independent subset with $2n+1$ components.

Proof. From (2.2) it is seen that each trace relation requires one component in which the exponent of $\hat{z}$ is 2 or more. Thus there are no trace relations among the components in which $n_3 = 0$ or 1. When $n_3 = 0$, there are $n+1$ sets (n_1, n_2) such that $n_1+n_2+n_3 = n$. When $n_3 = 1$, there are n such sets. Hence there are $2n+1$ components with $n_3 = 0$ or 1.

The linearly independent subset specified in the theorem gives unique status to the z axis. Two other linearly independent subsets may be obtained by choosing the x or y axis to have this status. Table 1 shows the independent subsets specified by the theorem for $n = 1, 2, 3$.

Table 1. Linearly independent subsets of $\mathscr{T}_n\hat{r}^n$

n	$n_1n_2n_3$	$\mathscr{T}_n\hat{x}^{n_1}\hat{y}^{n_2}\hat{z}^{n_3}$
1	1 0 0	$\hat{x}$
	0 1 0	$\hat{y}$
	0 0 1	$\hat{z}$
2	2 0 0	$3\hat{x}^2-1$
	1 1 0	$3\hat{x}\hat{y}$
	1 0 1	$3\hat{x}\hat{z}$
	0 2 0	$3\hat{y}^2-1$
	0 1 1	$3\hat{y}\hat{z}$
3	3 0 0	$15\hat{x}^3-9\hat{x}$
	2 1 0	$15\hat{x}^2\hat{y}-3\hat{y}$
	2 0 1	$15\hat{x}^2\hat{z}-3\hat{z}$
	1 2 0	$15\hat{x}\hat{y}^2-3\hat{x}$
	1 1 1	$15\hat{x}\hat{y}\hat{z}$
	0 3 0	$15\hat{y}^3-9\hat{y}$
	0 2 1	$15\hat{y}^2\hat{z}-3\hat{z}$

8.3. Comparison with $Y_n^m(\theta, \phi)$.

The functions in table 1 are closely related to the tesseral harmonics $Y_n^m(\theta, \phi)$, when the latter are expressed in cartesian form (Edmonds 1974, p124). The corresponding $Y_n^m(\theta, \phi)$ are best known as the angular part of the hydrogen atom wavefunctions (unnormalised) for p, d and f orbitals. However, there are significant differences. For $n = 2$, for example, table 1 lists the functions $3\hat{x}^2 - 1$ and $3\hat{y}^2 - 1$ in place of the usual d_{z^2} and $d_{x^2-y^2}$ functions, which are linear combinations of the former. In § 8.5 this linear transformation will be treated generally. At this point it seems worthwhile to summarise some major similarities and differences between the $\mathcal{T}_n\hat{r}^n$ and $Y_n^m(\theta, \phi)$ functions, in addition to those noted in § 7.1.

(i) Both functions are solutions to the same partial differential equation, the angular part of the Laplace equation.

(ii) Like the $\mathcal{T}_n\hat{r}^n$ components, $Y_n^m(\theta, \phi)$ can be derived in the form $\mathbf{A}^{(n)} \cdot n \cdot \hat{r}^n$, where $\mathbf{A}^{(n)}$ is a totally symmetric and traceless tensor. For this purpose one takes $\mathbf{A}^{(n)} = \boldsymbol{a}^n$, where $\boldsymbol{a}$ is a non-vanishing vector satisfying $\boldsymbol{a} \cdot \boldsymbol{a} = 0$ (Böttcher 1952, p86). Consequently $\boldsymbol{a}$ is complex, and $Y_n^m(\theta, \phi)$ is likewise complex. $\mathcal{T}_n\hat{r}^n$, by contrast, is real.

(iii) $Y_n^m(\theta, \phi)$ can be expressed as a product of functions of the form $f(\theta)g(\phi)$ according to (7.5), while this is not generally true for $\mathcal{T}_n\hat{r}^n$; for example $\mathcal{T}_2\hat{x}^2 = 3\hat{x}^2 - 1 = 3\sin^2\theta\cos^2\phi - 1$. It might be noted that the condition of separability of variables is usually imposed for convenience in deriving solutions to the Schrödinger equation for the hydrogen atom, necessarily resulting in solutions of the form $Y_n^m(\theta, \phi)$ (Pauling and Wilson 1935).

(iv) $Y_n^m(\theta, \phi)$ and $Y_n^{m'}(\theta, \phi)$, with $m \neq m'$, are orthogonal (Böttcher 1952, p473) while members of a linearly independent subset of $\mathcal{T}_n\hat{r}^n$ are not in general orthogonal (see § 8.6).

(v) Both $Y_n^m(\theta, \phi)$ and the linearly independent subset of $\mathcal{T}_n\hat{r}^n$ contain $2n+1$ components. Both sets thus constitute irreducible tensors, since they contain the minimum number of components which transform under rotations by linear combinations among themselves (Gray and Gubbins 1984, p477, p493).

8.4. $\mathcal{T}_n\hat{r}^n$ in terms of its linearly independent subset

Since $\mathcal{T}_n\hat{r}^n$ contains redundant components, we wish to express all components in terms of a linearly independent subset. The following theorem gives the necessary expression when the subset is chosen as in § 8.1, with the z axis as the unique axis.

Theorem. Any component of $\mathcal{T}_n\hat{r}^n$ is given by

$$\mathcal{T}_n\hat{x}^{n_1}\hat{y}^{n_2}\hat{z}^{n_3} = (-1)^\nu \sum_{m=0}^{\nu} \binom{\nu}{m} \mathcal{T}_n\hat{x}^{n_1+2m}\hat{y}^{n_2+2\nu-2m}\hat{z}^{n_3-2\nu} \tag{8.6}$$

where $\nu = [n_3/2]$, $n_1 + n_2 + n_3 = n$ and $\binom{\nu}{m} = \nu!/m!(\nu - m)!$.

Comment. The exponent of $\hat{z}$ in the summand of (8.6) is 0 or 1, according as n_3 is even or odd, respectively. Thus the sum includes only members of the linearly independent subset.

Proof. Let $T(n_1n_2n_3) = \mathcal{T}_n\hat{x}^{n_1}\hat{y}^{n_2}\hat{z}^{n_3}$. By introducing trace relations of the form (2.2), we reduce the third index to 0 or 1 in ν successive steps:

$$\begin{aligned} T(n_1n_2n_3) &= -T(n_1+2, n_2, n_3-2) - T(n_1, n_2+2, n_3-2) \\ &= [T(n_1+4, n_2, n_3-4) + T(n_1+2, n_2+2, n_3-4)] \\ &\quad + [T(n_1+2, n_2+2, n_3-4) + T(n_1, n_2+4, n_3-4)] \end{aligned}$$

$$= \dots$$

$$= (-1)^{\nu} \sum_{m=0}^{\nu} \binom{\nu}{m} T(n_1 + 2m, n_2 + 2\nu - 2m, n_3 - 2\nu).$$

Each substitution step doubles the number of terms and subtracts 2 from the third index. The binomial coefficient in the final summand is the number of different sequences of steps by which m increments of 2 are added to the first index and $(\nu - m)$ increments of 2 are added to the second index. All 2^{ν} terms are thus accounted for.

8.5. $Y_n^m(\theta, \phi)$ in terms of $\mathcal{T}_n\hat{r}^n$

The following theorem provides a means of generating the tesseral harmonics from the cartesian basis surface spherical harmonics.

Theorem. For $0 \le m \le n$,

$$Y_n^m(\theta, \phi) = \frac{1}{(n-m)!} \sum_{k=0}^{m} \mathrm{i}^{m-k} \binom{m}{k} \mathcal{T}_n \hat{x}^k \hat{y}^{m-k} \hat{z}^{n-m}. \tag{8.7}$$

Proof. From the theory of the gradients of r^{-1} (Hobson 1931, p134), one has

$$\nabla_3^{n-m} (\nabla_1 + \mathrm{i}\nabla_2)^m r^{-1} = (-1)^n (n-m)! r^{-n-1} Y_n^m(\theta, \phi). \tag{8.8}$$

Here a factor $(-1)^m$ appearing in Hobson's treatment is omitted in order to conform to common usage in the physics literature, where a factor $(-1)^m$ included in Hobson's definition of $P_n^m(\cos\theta)$ is omitted. By applying the binomial theorem and (6.1) to the left-hand side of (8.8), one obtains (8.7).

Comment. For harmonics of negative order we have (Hobson 1931, p90)

$$P_n^{-m}(\cos\theta) = (-1)^m \frac{(n-m)!}{(n+m)!} P_n^m(\cos\theta)$$

and hence, from (7.5),

$$Y_n^{-m}(\theta, \phi) = (-1)^m \frac{(n-m)!}{(n+m)!} Y_n^{m*}(\theta, \phi)$$

which extends (8.7) to negative orders.

The components of $\mathcal{T}_n\hat{r}^n$ in (8.7) are not all linearly independent. By introducing (8.6) into (8.7), a relation between $Y_n^m(\theta, \phi)$ and a linearly independent subset of $\mathcal{T}_n\hat{r}^n$ is obtained. The relation can be represented by a square transformation matrix of order $2n+1$, since there are $2n+1$ components in both basis sets. (The matrix is not, in general, unitary; hence the inverse transformation cannot be carried out by the conjugate transpose matrix.)

8.6. Values of $\mathcal{T}_n\hat{r}^n$ on the coordinate axes

The values of the components of $\mathcal{T}_n\hat{r}^n$ on the coordinate axes are easily obtained, and serve to locate certain nodes and extrema of the functions. We use (6.2) to evaluate the functions at $(x, y, z) = (1, 0, 0)$ on the x axis. The values on the y and z axes can then be obtained by cyclic permutation of indices. At the point of interest, all terms of the function vanish except the one for which $n_2 - 2m_2 = 0$ and $n_3 - 2m_3 = 0$. When n_2 or n_3 is odd, this condition cannot be met, and the function vanishes. For even values of n_2 and n_3, we set $r = x = 1$ in (6.2) and obtain

$$\mathcal{T}_n\hat{x}^{n_1}\hat{y}^{n_2}\hat{z}^{n_3}\Big]_{\hat{x}=1} = (-1)^{(n_2+n_3)/2}(n_2-1)!!(n_3-1)!! \times \sum_{m_1=0}^{[n_1/2]} (-1)^{m_1} \begin{bmatrix} n_1 \\ m_1 \end{bmatrix} (n+n_1-2m_1-1)!!$$

using the identity $(n-1)!! = \left[{n \atop n/2}\right]$ for even n. The value at $(-1, 0, 0)$ is, from (6.2),

$$\mathcal{T}_n\hat{x}^{n_1}\hat{y}^{n_2}\hat{z}^{n_3}\Big]_{\hat{x}=-1} = (-1)^{n_1}\mathcal{T}_n\hat{x}^{n_1}\hat{y}^{n_2}\hat{z}^{n_3}\Big]_{\hat{x}=1}.$$

Two special cases take a simple form which follows from (7.2). Since $P_n(1) = 1$, and, for even n, $P_n(0) = (-1)^{n/2}[(n-1)!!]^2/n!$ (Hobson 1931, p17), we find

$$\mathcal{T}_n\hat{x}^n\Big]_{\hat{x}=1} = n!$$
$$\mathcal{T}_n\hat{y}^n\Big]_{\hat{x}=1} = (-1)^{n/2}[(n-1)!!]^2 \qquad n \text{ even.}$$

8.7. Integrals involving $\mathcal{T}_n\hat{r}^n$

In this section we obtain a number of integrals which occur, for example, when expressions involving $\nabla^n r^{-1}$ are integrated over regions with spherical symmetry. The Laplace theorem of orthogonality of spherical harmonics of different degrees (Hobson 1931, p144) gives

$$\int_s \mathcal{T}_m\hat{r}^m\mathcal{T}_n\hat{r}^n ds = 0 \qquad m \neq n \tag{8.9}$$

where the integral is over the surface of the unit sphere and m, n are non-negative integers. Equation (8.9) means that all components vanish in the tensor of rank $m+n$ implied by the integral. For the special case $m = 0$, (8.9) becomes

$$\int_s \mathcal{T}_n\hat{r}^n \,\mathrm{d}s = 0 \qquad n = 1, 2, \ldots.$$

A theorem due to Hobson (1931, p156) gives

$$\int_s \hat{r}^m\mathcal{T}_n\hat{r}^n \,\mathrm{d}s = 0 \qquad m < n \text{ or } m+n \text{ odd}$$

where m and n are non-negative integers. The case where $m \geq n$ and $m+n$ is even is also covered by Hobson's theorem, but the explicit formula requires some derivation. This is supplied by the following.

Theorem. If m and n are non-negative integers with $m \geq n$ and $m+n$ even, then, with $m_1+m_2+m_3 = m$ and $n_1+n_2+n_3 = n$,

$$\int_s \hat{x}^{m_1}\hat{y}^{m_2}\hat{z}^{m_3}\mathscr{T}_n\hat{x}^{n_1}\hat{y}^{n_2}\hat{z}^{n_3}\,\mathrm{d}s$$
$$= \frac{2^{n+2}\pi(n+k)!m_1!m_2!m_3!}{k!(m+n+1)!}\sum_{k_1k_2k_3} g(k;k_1k_2k_3)$$
$$\times \sum_{j_1=0}^{[n_1/2]}\sum_{j_2=0}^{[n_2/2]}\sum_{j_3=0}^{[n_3/2]}(-1)^j(2n-2j-1)!!\begin{bmatrix} n_1 \\ j_1 \end{bmatrix}\begin{bmatrix} n_2 \\ j_2 \end{bmatrix}\begin{bmatrix} n_3 \\ j_3 \end{bmatrix}$$
$$\times g[j;\tfrac{1}{2}(m_1-n_1)+j_1-k_1, \tfrac{1}{2}(m_2-n_2)+j_2-k_2, \tfrac{1}{2}(m_3-n_3)+j_3-k_3] \tag{8.10}$$

where $k = \frac{1}{2}(m-n)$, $j = j_1+j_2+j_3$, and the g function is zero if any argument is negative or non-integral.

Comment. The theorem implies that the integral vanishes if any $m_i - n_i$ is odd ($i = 1, 2, 3$); i.e. if corresponding indices have opposite parity.

Proof. Hobson's theorem for this case states that, for any solid spherical harmonic $H_n(\boldsymbol{r})$ of degree n

$$\int_s \hat{x}^{m_1}\hat{y}^{m_2}\hat{z}^{m_3}H_n(\hat{\boldsymbol{r}})\,\mathrm{d}s = \frac{2^{n+2}\pi(n+k)!}{k!(m+n+1)!}\nabla^{2k}H_n(\nabla)x^{m_1}y^{m_2}z^{m_3} \tag{8.11}$$

where

$$\nabla^{2k} = (\nabla_1^2+\nabla_2^2+\nabla_3^2)^k = \sum_{k_1k_2k_3} g(k;k_1k_2k_3)\nabla_1^{2k_1}\nabla_2^{2k_2}\nabla_3^{2k_3}.$$

Let $H_n(\boldsymbol{r}) = \mathscr{T}_n\boldsymbol{r}^n$, so $H_n(\nabla) = \mathscr{T}_n\nabla_1^{n_1}\nabla_2^{n_2}\nabla_3^{n_3}$. One applies the latter to (8.11) to obtain (8.10), using (5.6) and recognising that, for $a+b+c = A+B+C$, $\nabla_1^A\nabla_2^B\nabla_3^C x^a y^b z^c$ vanishes unless $A = a$, $B = b$, and $C = c$, and is then equal to $a!b!c!$.

For the product of a pair of components of $\mathscr{T}_n\boldsymbol{r}^n$ we have the following integral theorem, which gives the condition for orthogonality.

Theorem. For non-negative integers a_i, n_i, ($i = 1, 2, 3$) such that $a_1+a_2+a_3 = n_1+n_2+n_3 = n$,

$$\int_s \mathscr{T}_n\hat{x}^{a_1}\hat{y}^{a_2}\hat{z}^{a_3}\mathscr{T}_n\hat{x}^{n_1}\hat{y}^{n_2}\hat{z}^{n_3}\,\mathrm{d}s$$
$$= \frac{4\pi a_1!a_2!a_3!}{2n+1}\sum_{m_1=0}^{[n_1/2]}\sum_{m_2=0}^{[n_2/2]}\sum_{m_3=0}^{[n_3/2]}(-1)^m(2n-2m-1)!!\begin{bmatrix} n_1 \\ m_1 \end{bmatrix}\begin{bmatrix} n_2 \\ m_2 \end{bmatrix}\begin{bmatrix} n_3 \\ m_3 \end{bmatrix}$$
$$\times g[m;\tfrac{1}{2}(a_1-n_1)+m_1, \tfrac{1}{2}(a_2-n_2)+m_2, \tfrac{1}{2}(a_3-n_3)+m_3] \tag{8.12}$$

where $m = m_1+m_2+m_3$ and the g function is zero if any argument is negative or non-integral.

Comment. The theorem implies that the integral vanishes if any $a_i - n_i$ is odd ($i = 1, 2, 3$); i.e. if corresponding indices have opposite parity.

Proof. Let $Y_n(\boldsymbol{r})$ be the nth-degree solid spherical harmonic

$$Y_n(\boldsymbol{r}) = \frac{(-1)^n r^{2n+1}}{n!} \nabla_1^{a_1} \nabla_2^{a_2} \nabla_3^{a_3} r^{-1} = \frac{r^n}{n!} \mathscr{T}_n \hat{x}^{a_1} \hat{y}^{a_2} \hat{z}^{a_3}.$$

If $Z_n(\boldsymbol{r})$ is any nth-degree solid spherical harmonic, Hobson's theorem (Hobson 1931, p157) becomes

$$\int_s Y_n(\hat{\boldsymbol{r}}) Z_n(\hat{\boldsymbol{r}})\, \mathrm{d}s = \frac{4\pi}{(2n+1)n!} \nabla_1^{a_1} \nabla_2^{a_2} \nabla_3^{a_3} Z_n(\boldsymbol{r}). \tag{8.13}$$

Let $Z_n(\boldsymbol{r}) = n! \mathscr{T}_n x^{n_1} y^{n_2} z^{n_3}$. Then (8.12) follows from (8.13), using (6.2).

For example, in $\mathscr{T}_2 \hat{x}^2$ and $\mathscr{T}_2 \hat{y}^2$ all indices are even, and (8.12) gives $-8\pi/5$ for the surface integral of the product. On the other hand, $\mathscr{T}_2 \hat{x}^2$ and $\mathscr{T}_2 \hat{x}\hat{y}$ are orthogonal, as the corresponding indices are of opposite parity.

By setting $a_i = n_i$ ($i = 1, 2, 3$) in (8.12) we have the following corollary, giving the integral which could be used to normalise the components of $\mathscr{T}_n \hat{\boldsymbol{r}}^n$.

Corollary. For non-negative integers n_i such that $n_1 + n_2 + n_3 = n$,

$$\begin{aligned}\int_s (\mathscr{T}_n \hat{x}^{n_1} \hat{y}^{n_2} \hat{z}^{n_3})^2\, \mathrm{d}s \\ &= \frac{4\pi n_1! n_2! n_3!}{2n+1} \sum_{m_1=0}^{[n_1/2]} \sum_{m_2=0}^{[n_2/2]} \sum_{m_3=0}^{[n_3/2]} (-1)^m \\ &\quad \times (2n-2m-1)!! \begin{bmatrix} n_1 \\ m_1 \end{bmatrix} \begin{bmatrix} n_2 \\ m_2 \end{bmatrix} \begin{bmatrix} n_3 \\ m_3 \end{bmatrix} g(m; m_1 m_2 m_3)\end{aligned} \tag{8.14}$$

where $m = m_1 + m_2 + m_3$.

Finally, by integrating (7.6) over the unit sphere, and using (2.1), we obtain a sum rule for the normalisation integrals:

$$\sum_{n_1 n_2 n_3} g(n; n_1 n_2 n_3) \int_s (\mathscr{T}_n \hat{x}^{n_1} \hat{y}^{n_2} \hat{z}^{n_3})^2\, \mathrm{d}s = \frac{4\pi(2n)!}{2^n}.$$

This result is obtained independently of (8.14), and may be useful as a check on the latter.

9. Electrostatic potentials of charges in a dielectric cavity

The method of traceless cartesian tensor forms for spherical harmonics will be used here to treat some problems of the electrostatic potential in a dielectric medium containing an arbitrary charge distribution in a spherical cavity. Such problems have been important in molecular theories of condensed phases (see, for example, Böttcher 1952, Felder and Applequist 1981), and the present formalism provides a convenient means of including higher-order effects in such theories. We are concerned with the potential and its gradients of all orders inside and outside the cavity.

9.1. Multipole expansion of potential in empty space

Let $\rho(\boldsymbol{s})$ be the electric charge density at point $\boldsymbol{s}$ for an arbitrary charge distribution located within a finite circumsphere in empty space. The nth-order multipole moment of the charge distribution about the origin is defined by

$$\boldsymbol{\mu}^{(n)} = \frac{1}{n!}\int_v \rho(\boldsymbol{s})\boldsymbol{s}^n \,\mathrm{d}v$$

where the integration is over the volume of the circumsphere. The potential $\phi_0(\boldsymbol{r})$ arising from $\rho(\boldsymbol{s})$ at any point $\boldsymbol{r}$ outside the circumsphere is given by the familiar multipole expansion (Böttcher *et al* 1973, p44):

$$\phi_0(\boldsymbol{r}) = \sum_{n=0}^{\infty}(-1)^n\boldsymbol{\mu}^{(n)}\cdot n\cdot\nabla^n r^{-1}. \tag{9.1}$$

Equation (9.1) is equivalent to an expansion in terms of the cartesian basis spherical harmonics, by virtue of (6.1). We introduce the traceless multipole moment $\mathbf{M}^{(n)} = \mathscr{T}_n\boldsymbol{\mu}^{(n)}$, and obtain from (5.4), (5.5) and (6.1) the useful identities

$$(-1)^n\boldsymbol{\mu}^{(n)}\cdot n\cdot\nabla^n r^{-1} = r^{-n-1}\mathbf{M}^{(n)}\cdot n\cdot\hat{\boldsymbol{r}}^n \tag{9.2}$$

$$(2n-1)!!\boldsymbol{\mu}^{(n)}\cdot n\cdot\nabla^n r^{-1} = \mathbf{M}^{(n)}\cdot n\cdot\nabla^n r^{-1}. \tag{9.3}$$

Either expression, substituted in (9.1), gives an alternative form to the spherical harmonic expansion (cf Applequist 1985). (9.2) demonstrates the well known fact that the nth-order multipole potential varies as r^{-n-1}, and in addition shows that the coefficient of r^{-n-1} is just the projection of $\mathbf{M}^{(n)}$ on $\boldsymbol{r}$, according to § 3.2.

9.2. Potentials and their gradients for arbitrary charge distribution

A spherical cavity of radius a is located inside a continuous medium of dielectric constant ε. Within the cavity is placed a charge distribution $\rho(\boldsymbol{r})$ which is zero outside a radius b from the cavity centre, with $b < a$, so that an arbitrarily thin charge-free region of the cavity exists next to the cavity wall.

9.2.1. Potentials in cavity and dielectric. The polarisation of the medium by the charges in the cavity produces a potential ϕ_{p1} outside the cavity and a potential ϕ_{p2} inside the cavity. Both potentials obey the Laplace equation throughout their respective regions, since, in the outer region, the charge density is zero everywhere, and, in the inner region, the superposition principle permits one to ignore the charge $\rho(\boldsymbol{r})$ because it does not contribute to ϕ_{p2}. Thus the potentials may be represented by spherical harmonic expansions (Böttcher 1952, p472), which we write as

$$\phi_{p1}(\boldsymbol{r}) = \sum_{n=0}^{\infty} r^{-n-1}\mathbf{A}^{(n)}\cdot n\cdot\hat{\boldsymbol{r}}^n \qquad r > a \tag{9.4}$$

$$\phi_{p2}(\boldsymbol{r}) = \sum_{n=0}^{\infty} r^{n}\mathbf{B}^{(n)}\cdot n\cdot\hat{\boldsymbol{r}}^n \qquad r < a \tag{9.5}$$

where $\mathbf{A}^{(n)}$ and $\mathbf{B}^{(n)}$ are totally symmetric and traceless tensors of rank n, to be determined by the boundary conditions at the cavity wall. The condition that $\phi_{\mathrm{p1}}(\boldsymbol{r}) \to 0$ as $r \to \infty$ has been incorporated in (9.4) by including spherical harmonics of negative degree only, and the condition that $\phi_{\mathrm{p2}}(\boldsymbol{r})$ remain finite at $r = 0$ has been incorporated in (9.5) by including spherical harmonics of non-negative degree only. The solution of the boundary value problem follows Böttcher (1952, p94) in most respects. The most notable distinction is our use of cartesian tensors in place of the spherical tensors of Böttcher's spherical harmonic expansions. Thus we obtain potentials expressed in terms of the cartesian multipole moments in a form that lends itself readily to the calculation of potential gradients of all orders.

Let the total potential outside the cavity be $\phi_1(\boldsymbol{r})$, and let that inside the cavity in the shell $b < r < a$ be $\phi_2(\boldsymbol{r})$. Then $\phi_1(\boldsymbol{r}) = \phi_0(\boldsymbol{r}) + \phi_{\mathrm{p1}}(\boldsymbol{r})$ and $\phi_2(\boldsymbol{r}) = \phi_0(\boldsymbol{r}) + \phi_{\mathrm{p2}}(\boldsymbol{r})$. The boundary conditions at the cavity wall are

$$\lim_{r\to a+} \phi_1(\boldsymbol{r}) = \lim_{r\to a-} \phi_2(\boldsymbol{r}) \tag{9.6}$$

$$\lim_{r\to a+} \varepsilon \frac{\partial \phi_1}{\partial r} = \lim_{r\to a-} \frac{\partial \phi_2}{\partial r}. \tag{9.7}$$

Application of these conditions using (9.1), (9.2), (9.4) and (9.5) leads to expressions of the form (4.1), from which $\mathbf{A}^{(n)}$ and $\mathbf{B}^{(n)}$ can be evaluated in terms of $\mathbf{M}^{(n)}$. Thus we find

$$\phi_{\mathrm{p1}}(\boldsymbol{r}) = (1-\varepsilon) \sum_{n=0}^{\infty} \left(\frac{n+1}{n\varepsilon + \varepsilon + n} \right) r^{-n-1} \mathbf{M}^{(n)} \cdot n \cdot \hat{\boldsymbol{r}}^{n} \tag{9.8}$$

$$\phi_{\mathrm{p2}}(\boldsymbol{r}) = (1-\varepsilon) \sum_{n=0}^{\infty} \left(\frac{n+1}{n\varepsilon + \varepsilon + n} \right) a^{-2n-1} r^{n} \mathbf{M}^{(n)} \cdot n \cdot \hat{\boldsymbol{r}}^{n}. \tag{9.9}$$

From (9.1), (9.2) and (9.8) we then have

$$\phi_1(\boldsymbol{r}) = \sum_{n=0}^{\infty} \left(\frac{2n+1}{n\varepsilon + \varepsilon + n} \right) r^{-n-1} \mathbf{M}^{(n)} \cdot n \cdot \hat{\boldsymbol{r}}^{n}. \tag{9.10}$$

9.2.2. Field gradients in dielectric. The mth-order electric field gradient in the dielectric outside the cavity is

$$\mathbf{E}_1^{(m)}(\boldsymbol{r}) = -\nabla^m \phi_1(\boldsymbol{r}). \tag{9.11}$$

Substituting (9.2) and (9.3) into (9.10) and applying (6.1) and (9.11), we find

$$\mathbf{E}_1^{(m)}(\boldsymbol{r}) = (-1)^{m+1} \sum_{n=0}^{\infty} \frac{2n+1}{(2n-1)!!(n\varepsilon + \varepsilon + n)} r^{-n-m-1} \mathbf{M}^{(n)} \cdot n \cdot \mathscr{T}_{n+m} \hat{\boldsymbol{r}}^{n+m}.$$

The right-hand side is a totally symmetric and traceless mth-rank tensor, as it must be to satisfy (9.11), whose right-hand side is the mth-order gradient of a potential which satisfies the Laplace equation. It is noteworthy that $\mathbf{E}_1^{(m)}(\boldsymbol{r})$ is independent of the cavity radius.

9.2.3. Reaction field gradients in cavity. The mth-order reaction field gradient inside the cavity is

$$\mathbf{E}_{\mathrm{R}}^{(m)}(\boldsymbol{r}) = -\nabla^m \phi_{\mathrm{p}2}(\boldsymbol{r}).$$

By applying (3.3) to (9.9) we obtain

$$\mathbf{E}_{\mathrm{R}}^{(m)}(\boldsymbol{r}) = (\varepsilon - 1)\sum_{n=m}^{\infty} \frac{(n+1)!}{(n-m)!(n\varepsilon+\varepsilon+n)} a^{-2n-1} r^{n-m} \mathbf{M}^{(n)} \cdot (n-m) \cdot \hat{\boldsymbol{r}}^{n-m}. \tag{9.12}$$

Again, the right-hand side is a totally symmetric and traceless mth-rank tensor, as required. At $r = 0$ only the $n = m$ term survives, so that

$$\mathbf{E}_{\mathrm{R}}^{(n)}(0) = \frac{(\varepsilon-1)(n+1)!}{(n\varepsilon+\varepsilon+n)} a^{-2n-1} \mathbf{M}^{(n)}. \tag{9.13}$$

Hence, at the cavity centre only the nth-order multipole moment contributes to the nth-order reaction field gradient. For $n = 1$, (9.13) becomes the known result for the dipole reaction field, $\mathbf{E}_{\mathrm{R}}^{(1)}(0) = [2(\varepsilon-1)/(2\varepsilon+1)a^3]\mathbf{M}^{(1)}$ (Böttcher 1952, p67).

9.3. Potentials and their gradients for point multipole in cavity

In molecular problems one may wish to treat the interactions among a number of separate charge distributions within the cavity. For this purpose it is convenient to assume that a given charge distribution is confined to an infinitesimal volume at point s within the cavity and possesses multipole moments $\bar{\boldsymbol{\mu}}^{(k)}$ about s, where the overbar indicates that the origin of the moment is not the cavity centre. In the following we consider the potentials due to a single point multipole moment $\bar{\boldsymbol{\mu}}^{(k)}$ of arbitrary order k. A summation over all k would give the potential of a general charge distribution in the cavity when s is chosen as origin, though this summation is omitted here for simplicity.

The multipole moments of the kth-order point multipole about the cavity centre are (Applequist 1984)

$$\boldsymbol{\mu}^{(n)} = \frac{k!}{n!}\sum_{P(n,k)} \boldsymbol{s}^{n-k}\bar{\boldsymbol{\mu}}^{(k)} \qquad n = k, k+1, \ldots \tag{9.14}$$

where the sum over $P(n,k)$ is the sum over all partitions of the n component indices into sets of k and $n-k$ indices. In the following sections we require also the relations

$$\mathbf{M}^{(n)} \cdot n \cdot \hat{\boldsymbol{r}}^n = \boldsymbol{\mu}^{(n)} \cdot n \cdot \mathscr{T}_n \hat{\boldsymbol{r}}^n \tag{9.15}$$

from (5.4), and

$$\frac{k!}{n!}\sum_{P(n,k)} \boldsymbol{s}^{n-k}\bar{\boldsymbol{\mu}}^{(k)} \cdot n \cdot \mathscr{T}_n \hat{\boldsymbol{r}}^n = \frac{1}{(n-k)!}\boldsymbol{s}^{n-k}\bar{\boldsymbol{\mu}}^{(k)} \cdot n \cdot \mathscr{T}_n \hat{\boldsymbol{r}}^n \tag{9.16}$$

from the fact that the sum on the left-hand side consists of $n!/k!(n-k)!$ identical terms. From (9.14) and (9.16) we have

$$\boldsymbol{\mu}^{(n)} \cdot n \cdot \mathscr{T}_n \hat{\boldsymbol{r}}^n = s^{n-k}\mathbf{D}_n^{(k)}(\hat{\boldsymbol{r}}, \hat{\boldsymbol{s}}) \cdot k \cdot \bar{\boldsymbol{\mu}}^{(k)} \tag{9.17}$$

where

$$\begin{aligned}\mathbf{D}_n^{(k)}(\hat{\boldsymbol{r}}, \hat{\boldsymbol{s}}) &\equiv \frac{1}{(n-k)!}\hat{\boldsymbol{s}}^{n-k} \cdot (n-k) \cdot \mathscr{T}_n \hat{\boldsymbol{r}}^n \\ &= r^n \frac{\partial^k}{\partial \boldsymbol{s}^k} s^n P_n(\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{s}})\end{aligned} \tag{9.18}$$

where the last equality follows from (7.7).

9.3.1. Potentials in cavity and in dielectric. Inserting (9.15) and (9.17) into (9.9) and (9.10), we obtain

$$\phi_1(\boldsymbol{r}) = \sum_{n=k}^{\infty} \left(\frac{2n+1}{n\varepsilon + \varepsilon + n} \right) r^{-n-1} s^{n-k} \mathbf{D}_n^{(k)}(\hat{\boldsymbol{r}}, \hat{\boldsymbol{s}}) \cdot k \cdot \overline{\boldsymbol{\mu}}^{(k)} \tag{9.19}$$

$$\phi_{\mathrm{p}2}(\boldsymbol{r}) = (1-\varepsilon) \sum_{n=k}^{\infty} \left(\frac{n+1}{n\varepsilon + \varepsilon + n} \right) a^{-2n-1} r^n s^{n-k} \mathbf{D}_n^{(k)}(\hat{\boldsymbol{r}}, \hat{\boldsymbol{s}}) \cdot k \cdot \overline{\boldsymbol{\mu}}^{(k)}. \tag{9.20}$$

The corresponding expressions for ϕ_0, $\phi_{\mathrm{p}1}$, and ϕ_2 are not required for what follows, but they may be obtained in a similar manner. Equations (9.19) and (9.20) may be cast in a useful form for computations using (7.1), (7.9) and (7.10) for $k = 0, 1, 2$, respectively, corresponding to the cases of a charge, dipole, and quadrupole located at s. For $k = 0$, (9.19) is identical to an expression derived earlier from results of Kirkwood (Felder and Applequist 1981, Kirkwood 1934).

9.3.2. Field gradients in dielectric. To obtain $\mathbf{E}_1^{(m)}$ we require the relation

$$\nabla^m r^{-n-1} \mathbf{D}_n^{(k)}(\hat{\boldsymbol{r}}, \hat{\boldsymbol{s}}) = (-1)^m r^{-n-m-1} \mathbf{D}_{n+m}^{(k+m)}(\hat{\boldsymbol{r}}, \hat{\boldsymbol{s}})$$

from (6.1) and (9.18). Hence, from (9.11) and (9.19),

$$\mathbf{E}_1^{(m)}(\boldsymbol{r}) = (-1)^m \sum_{n=k}^{\infty} \left(\frac{2n+1}{n\varepsilon + \varepsilon + n} \right) r^{-n-m-1} s^{n-k} \mathbf{D}_{n+m}^{(k+m)}(\hat{\boldsymbol{r}}, \hat{\boldsymbol{s}}) \cdot k \cdot \overline{\boldsymbol{\mu}}^{(k)}.$$

9.3.3. Reaction field gradients in cavity. $\mathbf{E}_{\mathrm{R}}^{(m)}$ for the point multipole case may be calculated from (9.12), using $\mathbf{M}^{(n)}$ obtained by applying $\mathscr{T}_n$ to both sides of (9.14). For the case $m = 1$ a more useful formula is obtained from the gradient of (9.20), using the relation

$$\nabla r^n \mathbf{D}_n^{(k)}(\hat{\boldsymbol{r}}, \hat{\boldsymbol{s}}) = r^{n-1}[(2n+1)\hat{\boldsymbol{r}} \mathbf{D}_n^{(k)}(\hat{\boldsymbol{r}}, \hat{\boldsymbol{s}}) - \mathbf{D}_{n+1}^{(k+1)}(\hat{\boldsymbol{r}}, \hat{\boldsymbol{s}})]$$

which follows from (8.4) and (9.18). Hence the reaction field is

$$\mathbf{E}_{\mathrm{R}}^{(1)}(\boldsymbol{r}) = (\varepsilon - 1) \sum_{n=k}^{\infty} \left(\frac{n+1}{n\varepsilon + \varepsilon + n} \right) a^{-2n-1} r^{n-1} s^{n-k}$$

$$\times [(2n+1)\hat{\boldsymbol{r}} \mathbf{D}_n^{(k)}(\hat{\boldsymbol{r}}, \hat{\boldsymbol{s}}) - \mathbf{D}_{n+1}^{(k+1)}(\hat{\boldsymbol{r}}, \hat{\boldsymbol{s}})] \cdot k \cdot \overline{\boldsymbol{\mu}}^{(k)}. \tag{9.21}$$

Higher gradients of the reaction field may be obtained by repeated application of (8.4) and (9.18) to (9.21), though I have not found a compact form for the mth-order gradient by this method. For the case $k = 1$, (9.21) corresponds to the dipole reaction field derived earlier (Felder and Applequist 1981) in terms of spherical coordinates.

10. Electrostatics of a dielectric sphere embedded in a dielectric medium

Consider a homogeneous dielectric with dielectric constant ε_1 in the presence of external charges which, with the apparent charges induced in the outer surface of the dielectric, give rise to a static potential $\phi_e(\boldsymbol{r})$ and the related gradients $\mathbf{E}_e^{(n)}(\boldsymbol{r}) = -\nabla^n\phi_e(\boldsymbol{r})$ within the dielectric. The potential is completely specified by the gradients at the origin by virtue of the Taylor series

$$\phi_e(\boldsymbol{r}) = -\sum_{n=0}^{\infty}\frac{1}{n!}\boldsymbol{r}^n\cdot n\cdot\mathbf{E}_e^{(n)}(0). \tag{10.1}$$

Now let a homogeneous dielectric sphere of radius a and dielectric constant ε_2 be embedded in the medium with its centre at the origin. It is assumed that the sphere is infinitely far from the boundaries of the outer dielectric, so that it has no effect on the external charges or apparent surface charges, and hence leaves all $\mathbf{E}_e^{(n)}(0)$ unchanged. In the following we will consider the field gradients that exist within the sphere, the multipole moments induced in the sphere, and the Lorentz internal (or 'effective') field gradients in the sphere.

10.1. Field gradients in embedded sphere

The presence of the embedded sphere gives rise to an additional potential $\phi_{s1}(\boldsymbol{r})$ outside the sphere and $\phi_{s2}(\boldsymbol{r})$ inside the sphere, so that the total potential outside is $\phi_1(\boldsymbol{r}) = \phi_e(\boldsymbol{r}) + \phi_{s1}(\boldsymbol{r})$ and that inside is $\phi_2(\boldsymbol{r}) = \phi_e(\boldsymbol{r}) + \phi_{s2}(\boldsymbol{r})$. As in § 9.2.1, these additional potentials may be expressed as the spherical harmonic expansions

$$\phi_{s1}(\boldsymbol{r}) = \sum_{n=0}^{\infty} r^{-n-1}\mathbf{C}^{(n)}\cdot n\cdot\hat{\boldsymbol{r}}^n \qquad r > a \tag{10.2}$$

$$\phi_{s2}(\boldsymbol{r}) = \sum_{n=0}^{\infty} r^{n}\mathbf{D}^{(n)}\cdot n\cdot\hat{\boldsymbol{r}}^n \qquad r < a \tag{10.3}$$

where the totally symmetric and traceless tensors $\mathbf{C}^{(n)}$ and $\mathbf{D}^{(n)}$ are to be determined by the boundary conditions at the surface of the sphere. These conditions are (9.6) and, in place of (9.7),

$$\lim_{r\to a+}\varepsilon_1\frac{\partial\phi_1}{\partial r} = \lim_{r\to a-}\varepsilon_2\frac{\partial\phi_2}{\partial r}.$$

Again, the boundary conditions, with (10.2) and (10.3), lead to two spherical harmonic expansions of the form (4.1), from which one finds, for $n = 1, 2, \ldots$,

$$\begin{aligned}\mathbf{C}^{(n)} &= a^{2n+1}\mathbf{D}^{(n)}\\ \mathbf{D}^{(n)} &= \frac{\varepsilon_2-\varepsilon_1}{(n-1)!(n\varepsilon_1+\varepsilon_1+n\varepsilon_2)}\mathbf{E}_e^{(n)}(0).\end{aligned} \tag{10.4}$$

Thus (10.1), (10.3) and (10.4) give an expansion for $\phi_2(\boldsymbol{r})$ whose coefficients of $\boldsymbol{r}^n$ are $-(1/n!)\mathbf{E}_2^{(n)}(0)$; hence

$$\mathbf{E}_2^{(n)}(0) = \frac{(2n+1)\varepsilon_1}{n\varepsilon_1+\varepsilon_1+n\varepsilon_2}\mathbf{E}_e^{(n)}(0) \qquad n = 1, 2, \ldots. \tag{10.5}$$

At any point $\boldsymbol{r}$ within the sphere we use the Taylor expansion

$$\mathbf{E}_2^{(n)}(\boldsymbol{r}) = \sum_{m=n}^{\infty} \frac{1}{(m-n)!} \boldsymbol{r}^{m-n} \cdot (m-n) \cdot \mathbf{E}_2^{(m)}(0)$$

$$= \sum_{m=n}^{\infty} \frac{(2m+1)\varepsilon_1}{(m-n)!(m\varepsilon_1 + \varepsilon_1 + m\varepsilon_2)} \boldsymbol{r}^{m-n} \cdot (m-n) \cdot \mathbf{E}_e^{(m)}(0). \tag{10.6}$$

If the external field is uniform, all gradients vanish except $\mathbf{E}_e^{(1)}(\boldsymbol{r}) = \mathbf{E}_e^{(1)}(0)$, and (10.6) reduces to the known relation $\mathbf{E}_2^{(1)}(\boldsymbol{r}) = [3\varepsilon_1/(2\varepsilon_1 + \varepsilon_2)]\mathbf{E}_e^{(1)}(0)$ (Böttcher 1952, p52).

10.2. Lorentz internal field gradients and induced multipole moments in sphere

The embedded sphere acquires the induced multipole moments $\mathbf{M}^{(n)}$ (traceless) in the presence of the external field gradients $\mathbf{E}_e^{(n)}$. The field acting on the sphere is the field due to all charges and polarisations outside the sphere, which is the Lorentz internal field, whose gradients we will denote as $\mathbf{E}_i^{(n)}(\boldsymbol{r})$. The internal field gradients may be regarded as consisting of two terms: (i) the cavity field gradients $\mathbf{E}_c^{(n)}$ present inside the spherical region when its material contents are removed; and (ii) the reaction field gradients $\mathbf{E}_R^{(n)}$ produced when the polarised sphere is returned to the cavity (cf Böttcher *et al* 1973). Thus

$$\mathbf{E}_i^{(n)}(0) = \mathbf{E}_c^{(n)}(0) + \mathbf{E}_R^{(n)}(0) \tag{10.7}$$

where $\mathbf{E}_c^{(n)}(0)$ is given by (10.5) with $\varepsilon_2 = 1$ and $\mathbf{E}_R^{(n)}(0)$ is given by (9.13) with $\varepsilon = \varepsilon_1$. A previous treatment (Applequist 1985) of the induced multipole moments of a dielectric sphere applies when $\mathbf{E}_i^{(n)}(0)$ is taken as the field of all charges outside the sphere, so that

$$\mathbf{M}^{(n)} = \frac{(\varepsilon_2 - 1)a^{2n+1}}{(n-1)!(n\varepsilon_2 + n + 1)} \mathbf{E}_i^{(n)}(0). \tag{10.8}$$

From (10.7) and (10.8) we find

$$\mathbf{M}^{(n)} = \frac{\varepsilon_1(\varepsilon_2 - 1)a^{2n+1}}{(n-1)!(n\varepsilon_1 + \varepsilon_1 + n\varepsilon_2)} \mathbf{E}_e^{(n)}(0) \tag{10.9}$$

and

$$\mathbf{E}_i^{(n)}(0) = \frac{\varepsilon_1(n\varepsilon_2 + n + 1)}{n\varepsilon_1 + \varepsilon_1 + n\varepsilon_2} \mathbf{E}_e^{(n)}(0). \tag{10.10}$$

The Lorentz internal field gradient at any point within the sphere may be obtained by a Taylor expansion similar to (10.6). It should be noted that $\mathbf{E}_i^{(n)}$ is not the same as $\mathbf{E}_2^{(n)}$, because the latter includes contributions from charges and polarisations both inside and outside the sphere. Thus (10.5) and (10.10) are identical when $\varepsilon_2 = 1$, i.e. when there is no matter in the sphere.

From (10.9) it is seen that the nth-order multipole moment is determined solely by the nth-order external field gradient at the origin. For the case $\varepsilon_1 = 1$, (10.9) is identical to the result for a dielectric sphere in a vacuum (Applequist 1985).

10.3. Lorentz internal field gradients in a homogeneous dielectric

If $\varepsilon_1 = \varepsilon_2 = \varepsilon$, then the entire system is a homogeneous dielectric. It is the internal field acting on a spherical region of such a system that was the subject of Lorentz' original investigation, whose object was to determine the field acting on the molecules of the medium. From (10.10) we have for this case

$$\mathbf{E}_i^{(n)}(0) = \frac{n\varepsilon + n + 1}{2n+1}\mathbf{E}_e^{(n)}(0). \tag{10.11}$$

For $n = 1$, (10.11) becomes the familiar Lorentz internal field $\mathbf{E}_i^{(1)}(0) = [(\varepsilon+2)/3]\mathbf{E}_e^{(1)}(0)$ (Böttcher 1952, p177). For $n = 2$, (10.11) becomes $\mathbf{E}_i^{(2)}(0) = [(2\varepsilon + 3)/5]\mathbf{E}_e^{(2)}(0)$, which is equivalent to a result obtained by Lorentz (1904, p214).

The results obtained here are rigorous for continuous media in static electric fields, and will have approximate validity in some time-dependent fields. However, it should be noted that a quantity such as $\nabla \times \mathbf{E}_i^{(1)}$, which is of interest in electrodynamics, vanishes in a static field, and therefore cannot be obtained from (10.11).

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