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Multipole expansions in four dimensions

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Abstract. In this paper we consider four-dimensional electrostatics. In 4D the electrostatic multipole moment of order l ($l=0, \frac{1}{2}, 1\ldots$) is a tensor with $(2l+1)^2$ independent components. We derive the multipole expansions for the potential due to an arbitrary distribution of charge, and for the energy of a charge distribution in a spatially non-uniform external electric field. We also derive the multipole expansion for the interaction energy of two rigid, non-overlapping charge distributions. The results are expressed in both Cartesian tensor and hyperspherical tensor forms.

The transformation properties of the moments, under the symmetry operations of the 4D rotation–reflection group O_4, and under translation of the coordinate axis system, are also derived.

1. Introduction

Problems in electrostatics generally involve computing either (a) the electric potential $\phi(\boldsymbol{r})$ or field $\boldsymbol{E}(\boldsymbol{r}) = -\nabla\phi$ produced by a charge distribution $\rho(\boldsymbol{r})$, or (b) the interaction energy u of a charge distribution with a field, generated either by a second distribution, or imposed externally in some essentially arbitrary specified fashion. In either case, provided spatial variations in $\boldsymbol{E}(\boldsymbol{r})$ are sufficiently weak on the scale of length that characterises $\rho(\boldsymbol{r})$, one can employ electrostatic *multipole expansions* to calculate $\boldsymbol{E}(\boldsymbol{r})$ (case (a)) or u (case (b)) (Buckingham 1967, 1978, Gray 1968, 1976, Gray and Gubbins 1983).

In the multipole expansion of u the interaction energy is decomposed into a succession of terms representing the interaction of the nth multipole moment of the charge distribution with the nth derivative of the potential ($(n-1)$th derivative of the field), evaluated at some point within the distribution. Such a series may only be asymptotically convergent if $\rho(\boldsymbol{r})$ does not fall strictly to zero outside some region of space (Jansen 1958); usually, however, it is a valid approximation to retain only a few terms (and sometimes only the leading term) of the multipole series. For example, at separations of chemical or physical interest, the anisotropic component of the electrostatic interaction energy between two CO_2 molecules is well represented by the quadrupole–quadrupole energy.

Calculations using the multipole expansion are often quite simple in practice. This is true even of high-order terms in the series if one uses spherical tensor methods (Gray 1968, 1976, Gray and Gubbins 1983) rather than the more familiar Cartesian tensor formalism (Buckingham 1967, 1978, Gray and Gubbins 1983).

Multipole expansions in three dimensions (3D) are well known. It is of interest, both intrinsically and in statistical mechanics, to consider other dimensions d, e.g.

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$d=1,2,4$. For $d=1$ the potential of a charge varies as r, and the expansions are trivial and terminate; for example, the only non-vanishing two-body electrostatic interaction energies are the charge–charge and charge–dipole terms. In 2D Joslin and Gray (1983) have recently derived the expansions for (a) the potential outside a given charge distribution; (b) the interaction energy of a rigid charge distribution with a given external field; and (c) the interaction energy of two non-overlapping rigid charge distributions, expressing the results in both Cartesian tensor and circular tensor forms. They found interesting differences from the 3D case. For example, in 2D, in any order l the multipole moment has at most *two* independent components; in 3D this number increases with l (as $2l+1$). Further, they showed that in 2D there is an *infinity* of preferred relative orientations for two interacting multipoles, which implies that in some respects, at least, the physics of 2D fluids and lattices may differ appreciably from that of their 3D analogues.

In this paper we derive the analogous results in *four* dimensions. The results are of mathematical interest in their own right: we find that the special functions which take the place of the multipole–multipole coupling tensors $\boldsymbol{T}^{(l)}(\hat{\boldsymbol{r}})$ and $e^{-il\lambda\theta}$ (in 2D) and $\boldsymbol{P}^{(l)}(\hat{\boldsymbol{r}})$ and $Y_{lm}(\theta\phi)$ (in 3D) (see Joslin and Gray 1983) are the tensor Chebyshev polynomials of the second kind, $\boldsymbol{U}^{(2l)}(\hat{\boldsymbol{r}})$, and the generalised, or hyperspherical, harmonics, $D^{l}_{mn}(\phi\theta\chi)$. (Here $\boldsymbol{T}^{(l)}$ is the tensor Chebyshev polynomial of the first kind, $\boldsymbol{P}^{(l)}$ is the tensor Legendre polynomial, and $e^{-il\lambda\theta}$ and $Y_{lm}(\theta\phi)$ are the circular and spherical harmonics, respectively.) The lth-order multipole moment in 4D is also expressed in terms of these functions, and is shown to have $(2l+1)^2$ ($l=0, \frac{1}{2}, 1\ldots$) independent components in general.

Our results can also be used as a starting-point in the calculation of thermodynamic and structural properties of 4D multipolar lattices and fluids. We can investigate, for example, whether there is a change in the nature of an orientational phase transition on a lattice, or in the dielectric properties of a fluid, as the dimensionality is increased from $d=2$ to $d=3$ to $d=4$. Apart from the intrinsic interest of studies in dimensions other than $d=3$, such calculations may provide a basis within which to calculate various properties of 3D systems using dimensional perturbation theory (Fisher 1974, Wilson 1979) about $d=4$ or $d=2$. (In 4D critical exponents are trivially obtainable, it being generally accepted that they have their classical, or mean-field, values; in 2D exact solutions (Baxter 1982) and more reliable computer simulation results (Occelli *et al* 1978, Bossis and Brot 1981, and references therein) are sometimes available.)

2. Solution of the 4D Laplace equation

The electrostatic potential $\phi(\boldsymbol{r})$ at a source-free point $\boldsymbol{r}=(r_1, r_2, r_3, r_4)$ satisfies the 4D Laplace equation

$$\nabla^2\phi=\sum_{\alpha=1}^{4}\frac{\partial^2\phi}{\partial r_\alpha^2}=0. \tag{2.1}$$

To solve (2.1) we transform from the Cartesian set (r_1, r_2, r_3, r_4) to polar coordinates (r, θ, ϕ, χ):

$$r_1=r\sin\tfrac{1}{2}\theta\sin\tfrac{1}{2}(\phi-\chi), \qquad r_2=r\sin\tfrac{1}{2}\theta\cos\tfrac{1}{2}(\phi-\chi),$$
$$r_3=r\cos\tfrac{1}{2}\theta\sin\tfrac{1}{2}(\phi+\chi), \qquad r_4=r\cos\tfrac{1}{2}\theta\cos\tfrac{1}{2}(\phi+\chi). \tag{2.2}$$

The r_α (with $r=1$) are the usual quaternion, or Euler–Rodrigues, parameters (Casimir 1931, Goldstein 1980, Biedenharn and Louck 1981, Gray and Gubbins 1983). The unit hypersphere is covered once if we allow

$$\begin{aligned} &0 \leqslant \phi < 2\pi, \\ &0 \leqslant \theta \leqslant \pi \qquad \textit{and} \qquad 2\pi \leqslant \theta \leqslant 3\pi, \\ &0 \leqslant \chi < 2\pi, \end{aligned} \tag{2.3}$$

the first and second ranges of θ covering, respectively, the two hemispheres $r_4 > 0$ and $r_4 < 0$ (Biedenharn and Louck 1981). There is thus a *two-to-one* correspondence between points on the 4D hypersphere and the configurations of a rigid body in 3D specified by the set of Euler angles (ϕ, θ, χ).

For angular parametrisations alternative to (2.2) see e.g. Biedenharn and Louck (1981). While the use of Euler angles is not encountered in the literature as commonly as the usual spherical polar coordinate formulation, it offers the distinct advantage of generating solutions of Laplace's equation in terms of the 3D rotation matrices, or generalised spherical harmonics (*vide infra*). The properties of these functions are of course well known from a study of the 3D rotation group (Brink and Satchler 1968).

In polar coordinates (2.1) reads

$$\nabla_r^2\phi + (4/r^2)\nabla_\Omega^2\phi = 0, \tag{2.4}$$

where the radial and angular parts of ∇^2 are given by

$$\nabla_r^2 = \frac{1}{r^3}\frac{\partial}{\partial r} r^3 \frac{\partial}{\partial r}, \tag{2.5}$$

and

$$\nabla_\Omega^2 = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial\chi^2} - 2\cos\theta\frac{\partial^2}{\partial\phi\,\partial\chi}\right). \tag{2.6}$$

The angular Laplacian (2.6) satisfies $\nabla_\Omega^2 = -\boldsymbol{L}^2$, where $\boldsymbol{L}^2$ is the operator for *the square of the total angular momentum of a rigid body in three dimensions.* The eigenfunctions of ∇_Ω^2 are immediately deduced to be the generalised spherical harmonics (hyperspherical harmonics) $D^l_{mn}(\Omega) \equiv D^l_{mn}(\phi\theta\chi)$ (Hund 1928, Casimir 1931, Gray and Gubbins 1983):

$$\nabla_\Omega^2 D^l_{mn}(\Omega) = -l(l+1)D^l_{mn}(\Omega). \tag{2.7}$$

In 3D the $D^l_{mn}(\Omega)$ are the transformation matrices for the spherical harmonics $Y_{lm}(\theta\phi)$ (Rose 1957, Brink and Satchler 1968, Gray and Gubbins 1983; we use the definition of $D^l_{mn}(\Omega)$ of these authors). In 4D the $D^l_{mn}(\Omega)$ furnish a *complete* set of spherical harmonics if we allow half-integral as well as integral values of l; this corresponds to the fact that in 4D the identity operation is rotation through 4π, rather than 2π, radians (this is evident from (2.2)).

We now seek solutions of (2.4) in the form $\phi = r^k D^l_{mn}(\Omega)$. We find using (2.7) that either $k = 2l$ or $k = -2(l+1)$. The general solution is therefore

$$\phi(r,\Omega) = \sum_{lmn} a_{lmn} r^{2l} D^l_{mn}(\Omega) + \sum_{lmn} b_{lmn} r^{-2(l+1)} D^l_{mn}(\Omega), \tag{2.8}$$

where a_{lmn} and b_{lmn} are arbitrary constants. (In (2.8) and all subsequent equations it is understood that Σ_l implies a summation over the values $l = 0, \frac{1}{2}, 1, \ldots, \infty$.)

The potential of a point charge cannot depend on Ω, and must therefore be given, to within a constant, by

$$\phi(r) = q/r^2, \tag{2.9}$$

with this equation defining the unit of charge.

3. Multipole expansion of the potential outside a charge distribution

We refer to figure 1. The potential at the external point P due to the charge distribution q_i, $i = 1, 2, \ldots, N$, is, from (2.9),

$$\phi(\boldsymbol{r}) = \sum_{i=1}^{N} q_i/(\boldsymbol{r}-\boldsymbol{r}_i)^2. \tag{3.1}$$

We make a Taylor expansion of $(\boldsymbol{r}-\boldsymbol{r}_i)^{-2}$ about the origin O (chosen arbitrarily):

$$\phi(\boldsymbol{r}) = \sum_{i=1}^{N} q_i \sum_n \frac{(-)^n}{n!} r_{i\alpha} \ldots r_{i\nu} \nabla_\alpha \ldots \nabla_\nu (1/r^2). \tag{3.2}$$

In (3.2) there are n factors $\nabla_\alpha \ldots \nabla_\nu$, α etc $= 1, 2, 3$ or 4, and the usual summation convention is employed. (In (3.2) and all subsequent equations it is understood that Σ_n implies a summation over the values $n = 0, 1, 2, \ldots, \infty$.)

We can show that

$$\nabla_\alpha \ldots \nabla_\nu (1/r^2) = (-)^n n!\, r^{-(n+2)} U^{(n)}_{\alpha\ldots\nu}(\hat{\boldsymbol{r}}), \tag{3.3}$$

where $U^{(n)}_{\alpha\ldots\nu}(\hat{\boldsymbol{r}})$ is a component of the tensor Chebyshev polynomial $\boldsymbol{U}^{(n)}(\hat{\boldsymbol{r}})$, which is defined so that

$$\begin{aligned} &U^{(0)}(\hat{\boldsymbol{r}}) = 1, && \boldsymbol{U}^{(1)}(\hat{\boldsymbol{r}}) = 2\hat{\boldsymbol{r}}, \\ &\boldsymbol{U}^{(2)}(\hat{\boldsymbol{r}}) = 4\hat{\boldsymbol{r}}\hat{\boldsymbol{r}} - \mathbf{1}, && \boldsymbol{U}^{(3)}(\hat{\boldsymbol{r}}) = 8\hat{\boldsymbol{r}}\hat{\boldsymbol{r}}\hat{\boldsymbol{r}} - 4\hat{\boldsymbol{r}}\mathbf{1}, \\ &\boldsymbol{U}^{(4)}(\hat{\boldsymbol{r}}) = 16\hat{\boldsymbol{r}}\hat{\boldsymbol{r}}\hat{\boldsymbol{r}}\hat{\boldsymbol{r}} - 12\hat{\boldsymbol{r}}\hat{\boldsymbol{r}}\mathbf{1} + \mathbf{11}, \end{aligned} \tag{3.4}$$

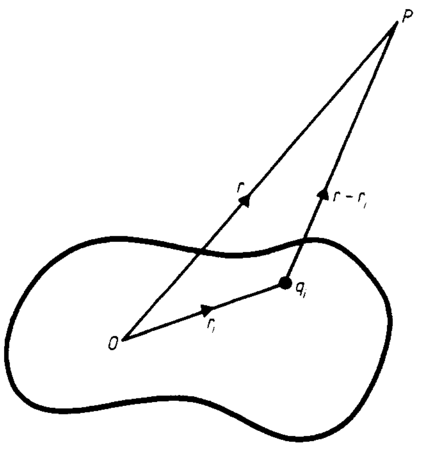

Figure 1. Geometry for the derivation of the multipole expansion, about the origin O, of the electrostatic potential at the point P external to the charge distribution q_i.

etc, and in general analogously to the Chebyshev polynomial of the second kind of degree n, $U_n(x)$ (Gradshteyn and Ryzhik 1965). In (3.4) $\hat{\boldsymbol{r}} \equiv \boldsymbol{r}/r$ is the unit vector along $\boldsymbol{r}$ and $\mathbf{1}$ is the unit tensor of rank 2. A normalised permutation of the indices is implied where appropriate: thus in $\boldsymbol{U}^{(3)}$, $(\hat{\boldsymbol{r}}\mathbf{1})_{\alpha\beta\gamma} \equiv \frac{1}{3}(\hat{r}_\alpha \delta_{\beta\gamma} + \hat{r}_\beta \delta_{\alpha\gamma} + \hat{r}_\gamma \delta_{\alpha\beta})$. For $n \geqslant 2$ the tensors $U^{(n)}_{\alpha\ldots\nu}$ are symmetric in any pair of indices; also, from (3.3), they are traceless, since $\nabla^2(1/r^2) = 0$.

Equation (3.3) is the 4D analogue of the 2D and 3D results

$$\begin{aligned} \nabla_\alpha \ldots \nabla_\nu \log r &= (-)^{n-1}(n-1)!\, r^{-n} T^{(n)}_{\alpha\ldots\nu}(\hat{\boldsymbol{r}}) \qquad (2\text{D}), \\ \nabla_\alpha \ldots \nabla_\nu (1/r) &= (-)^n n!\, r^{-(n+1)} P^{(n)}_{\alpha\ldots\nu}(\hat{\boldsymbol{r}}) \qquad (3\text{D}), \end{aligned} \tag{3.5}$$

in which $T^{(n)}_{\alpha\ldots\nu}(\hat{\boldsymbol{r}})$ is a tensor Chebyshev polynomial of the first kind (Joslin and Gray 1983), and $P^{(n)}_{\alpha\ldots\nu}(\hat{\boldsymbol{r}})$ is a tensor Legendre polynomial (Kielich 1965). (In the more general case of a d-dimensional space, the characteristic functions are tensor polynomials defined analogously to the Gegenbauer polynomials $C_n^{d/2-1}(x)$.)

We can therefore write (3.2) as

$$\phi(\boldsymbol{r}) = \sum_n r^{-(n+2)} \boldsymbol{U}^{(n)}(\hat{\boldsymbol{r}}) \bullet \boldsymbol{M}^{(n/2)}, \tag{3.6}$$

where the large dot $\bullet$ denotes a full (n-fold) tensor contraction, and the multipole moment $\boldsymbol{M}^{(n/2)}$ is defined as $\boldsymbol{M}^{(n/2)} = \Sigma_{i=1}^N q_i \boldsymbol{r}_i^n$, or more explicitly

$$M^{(n/2)}_{\alpha\ldots\nu} = \sum_i q_i r_{i\alpha} \ldots r_{i\nu}. \tag{3.7}$$

(The reason we choose to label the nth-rank moment with the superscript $\frac{1}{2}n$, rather than n, is to obtain closer correspondence with the definitions of the hyperspherical tensor multipole moments (see below).)

We can alternatively define a moment

$$Q^{(n/2)}_{\alpha\ldots\nu} = \sum_i q_i r_i^n U^{(n)}_{\alpha\ldots\nu}(\hat{\boldsymbol{r}}_i), \qquad n = 0, 1, 2 \ldots, \tag{3.8}$$

or, equivalently,

$$Q^{(l)}_{\alpha\ldots\nu} = \sum_i q_i r_i^{2l} U^{(2l)}_{\alpha\ldots\nu}(\hat{\boldsymbol{r}}_i), \qquad l = 0, \tfrac{1}{2}, 1 \ldots, \tag{3.9}$$

and then

$$\phi(\boldsymbol{r}) = \sum_n \frac{1}{2^n r^{n+2}} \boldsymbol{U}^{(n)}(\hat{\boldsymbol{r}}) \bullet \boldsymbol{Q}^{(n/2)} = \sum_l \frac{1}{2^{2l} r^{2(l+1)}} \boldsymbol{U}^{(2l)}(\hat{\boldsymbol{r}}) \bullet \boldsymbol{Q}^{(l)}. \tag{3.10}$$

The equality of (3.6) and (3.10) follows from the observation that $U^{(n)}_{\alpha\ldots\nu}$ is traceless, as noted earlier, i.e.

$$\boldsymbol{U}^{(n)}(\hat{\boldsymbol{r}}) : \mathbf{1} = 0, \qquad n \geqslant 2. \tag{3.11}$$

It is then only necessary to note that the coefficient of x^n in $U_n(x)$ is 2^n (Gradshteyn and Ryzhik 1965).

The definition (3.9) has the advantage that all moments for which $l \geqslant 1$ contract with the unit tensor to give zero: thus the quadrupole moment $\boldsymbol{Q}^{(1)}$ is traceless, the octopole $\boldsymbol{Q}^{(3/2)}$ is traceless in any pair of indices, etc. We can then show (appendix 1) that the lth-order multipole moment $\boldsymbol{Q}^{(l)}$ has at most $(2l+1)^2$ independent components. (Remember that $\boldsymbol{Q}^{(l)}$ has *order* l but *rank* $2l$.)

The derivation of the multipole expansion of ϕ in hyperspherical tensor form is straightforward if we write

$$(\boldsymbol{r}-\boldsymbol{r}_i)^{-2}=r^{-2}[1-2(r_i/r)\hat{\boldsymbol{r}}_i\cdot\hat{\boldsymbol{r}}+(r_i/r)^2]^{-1}, \tag{3.12}$$

and note that

$$(1-2tx+t^2)^{-1}=\sum_n U_n(x)t^n \tag{3.13}$$

(Gradshteyn and Ryzhik 1965). Then we get

$$\phi(r,\Omega)=\sum_n \frac{1}{r^{n+2}}\sum_i q_i r_i^n U_n(\hat{\boldsymbol{r}}_i\cdot\hat{\boldsymbol{r}})=\sum_l \frac{1}{r^{2(l+1)}}\sum_i q_i r_i^{2l} U_{2l}(\hat{\boldsymbol{r}}_i\cdot\hat{\boldsymbol{r}}). \tag{3.14}$$

To proceed further, note that the unit vectors $\hat{\boldsymbol{r}}_i$ and $\hat{\boldsymbol{r}}$ are each specified by a set of three Euler angles, $(\phi_i, \theta_i, \chi_i)\equiv\Omega_i$ and $(\phi, \theta, \chi)\equiv\Omega$. Suppose that to bring these two vectors into coincidence we need to apply a rotation through an angle ψ about the direction $\hat{\boldsymbol{n}}$ in the three-space spanned by ϕ, θ and χ. The closure relations for the unitary rotation matrices D^l yield (Brink and Satchler 1968)

$$\sum_{mn} D^l_{mn}(\Omega_i)D^l_{mn}(\Omega)^*=\sum_{mn} D^l_{mn}(\Omega_i)D^l_{nm}(\Omega^{-1})$$
$$=\operatorname{Tr} D^l(\Omega_i\Omega^{-1})=\operatorname{Tr} D^l(\psi, \hat{\boldsymbol{n}}). \tag{3.15a}$$

The trace of the rotation matrix depends only on the angle of rotation (Biedenharn and Louck 1981):

$$\operatorname{Tr} D^l(\psi, \hat{\boldsymbol{n}})=\sin(2l+1)\tfrac{1}{2}\psi/\sin\tfrac{1}{2}\psi=U_{2l}(\cos\tfrac{1}{2}\psi). \tag{3.15b}$$

We next note that from (2.2)

$$\hat{\boldsymbol{r}}_i\cdot\hat{\boldsymbol{r}}=\tfrac{1}{2}\sum_{mn} D^{1/2}_{mn}(\Omega_i)D^{1/2}_{mn}(\Omega)^*, \tag{3.16a}$$

while as a special case of (3.15a) and (3.15b), taking $l=\frac{1}{2}$,

$$\tfrac{1}{2}\sum_{mn} D^{1/2}_{mn}(\Omega_i)D^{1/2}_{mn}(\Omega)^*=\cos\tfrac{1}{2}\psi. \tag{3.16b}$$

Therefore we have

$$\hat{\boldsymbol{r}}_i\cdot\hat{\boldsymbol{r}}=\cos\tfrac{1}{2}\psi. \tag{3.16c}$$

Combining (3.14), (3.15a), (3.15b) and (3.16c), we finally deduce that

$$\phi(r,\Omega)=\sum_{lmn} r^{-2(l+1)}D^l_{mn}(\Omega)^*Q^l_{mn}, \tag{3.17}$$

where we have defined the *hyperspherical tensor multipole moments*

$$Q^l_{mn}=\sum_i q_i r_i^{2l} D^l_{mn}(\Omega_i). \tag{3.18}$$

In 4D the characteristic functions which enter the moment definition (3.18) and the potential expansion (3.17) are the hyperspherical harmonics $D^l_{mn}(\phi\theta\chi)$. In 2D and 3D the corresponding results involve the circular harmonics $e^{il\lambda\theta}$, and spherical harmonics $Y_{lm}(\theta\phi)$, respectively (Joslin and Gray 1983, Gray and Gubbins 1983).

From (3.18) we see immediately, in agreement with our earlier conclusion, that the lth multipole moment has at most $(2l+1)^2$ independent components.

The relationship between the hyperspherical tensor and Cartesian tensor forms of the moments is discussed in appendix 2.

The transformation properties of the Q^l_{mn} under the symmetry operations of the 4D rotation–reflection group O_4, and under translation of the coordinate axis system, are discussed in appendix 3. The Q^l_{mn} (and also the $\boldsymbol{Q}^{(l)}$) are irreducible tensors with respect to O_4. Note that

$$Q^{l*}_{mn} = (-)^{m-n} Q^l_{-m-n}. \tag{3.18a}$$

The relation (3.17) can also be derived directly using electrostatic and symmetry arguments (analogous to those used in 3D by Gray (1976) and in 2D by Joslin and Gray (1983)). We expand the angle dependence of $(\boldsymbol{r}-\boldsymbol{r}_i)^{-2}$ as a double series in the products $D^{l_1}_{m_1n_1}(\Omega_i)D^{l_2}_{m_2n_2}(\Omega)^*$ (remembering that the D^l_{mn} furnish a complete set of periodic functions in 4D). Because $(\boldsymbol{r}-\boldsymbol{r}_i)^{-2}$ is invariant under rotations, only the combinations $\Sigma_{mn} D^l_{mn}(\Omega_i)D^l_{mn}(\Omega)^*$ can occur (cf (3.15a)). Since $(\boldsymbol{r}-\boldsymbol{r}_i)^{-2}$ satisfies the Laplace equations in $\boldsymbol{r}$ and $\boldsymbol{r}_i$, and because the solutions depend on r and r_i as in (2.8), the expansion must have the form

$$(\boldsymbol{r}-\boldsymbol{r}_i)^{-2} = \sum_{lmn} A_l(r_i^{2l}/r^{2(l+1)})D^l_{mn}(\Omega_i)D^l_{mn}(\Omega)^* \tag{3.19}$$

for the region $r > r_i$; we have used the boundary conditions that $(\boldsymbol{r}-\boldsymbol{r}_i)^{-2} \to r^{-2}$ for $r_i \to 0$ or $r \to \infty$. The dimensionless constant A_l is found by considering the case where $\boldsymbol{r}_i$ is parallel to $\boldsymbol{r}$. Equation (3.19) reduces to

$$(r-r_i)^{-2} = \sum_l (2l+1)A_l(r_i^{2l}/r^{2(l+1)}), \tag{3.20}$$

whereas direct expansion of the LHS of (3.20) gives

$$(r-r_i)^{-2} = \sum_l (2l+1)(r_i^{2l}/r^{2(l+1)}). \tag{3.21}$$

Comparison of (3.20) and (3.21) gives $A_l = 1$. Substitution of (3.19) in (3.1) then yields (3.17).

If the system of charges q_i possesses elements of symmetry, some moments vanish. If there is a centre of inversion (twofold rotational axis), all moments with half-integral values of l vanish; we can have only charge ($l=0$), quadrupole ($l=1$), hexadecapole ($l=2$) moments, etc. This is readily seen from the definition of the Cartesian moments in terms of Chebyshev polynomials, or by noting that under inversion the Q^l_{mn} transform according to

$$Q^l_{mn} \to Q^l_{m'n'} = (-)^{2l} Q^l_{mn} \tag{3.22}$$

(see appendix 3; note that in (3.22) and all successive transformation equations, we use Schouten's kernel-index notation (Schouten 1954), where the components of a tensor which are Q^l_{mn} in frame S are denoted $Q^l_{m'n'}$ in frame S'). If there is *axial* symmetry, i.e. if the charge distribution is invariant under an arbitrary rotation about some axis $\hat{\boldsymbol{n}}$, then we have

$$Q^l_{mn} = Q^l D^l_{mn}(\Omega_{\hat{n}}), \tag{3.23}$$

where Q^l is the *unique* multipole moment of order l, and $\Omega_{\hat{n}} = (\phi_{\hat{n}}, \theta_{\hat{n}}, \chi_{\hat{n}})$ specifies the direction of $\hat{\boldsymbol{n}}$ in four-space (see appendix 3). Taking the trace of both sides of

(3.23) in the principal axis system $\Omega_{\hat{n}}=0$, using (3.15*b*) and the definition (3.18), we find

$$Q^l=(2l+1)^{-1}\sum_i q_i r_i^{2l}U_{2l}(\cos\tfrac{1}{2}\psi_i), \tag{3.24}$$

where ψ_i is the angle between $\boldsymbol{r}_i$ and the symmetry axis $\hat{\boldsymbol{n}}$. In this case (3.17) simplifies to

$$\phi(r,\psi)=\sum_l (Q^l/r^{2(l+1)})U_{2l}(\cos\tfrac{1}{2}\psi), \tag{3.25}$$

where ψ is the angle between $\boldsymbol{r}$ and $\hat{\boldsymbol{n}}$.

The Cartesian analogue of (3.23) is

$$Q^{(l)}_{\alpha\ldots\nu}=Q^l U^{(2l)}_{\alpha\ldots\nu}(\hat{\boldsymbol{n}}) \tag{3.26}$$

(see appendix 3). In axial symmetry (3.10) therefore simplifies to

$$\phi(r,\hat{\boldsymbol{r}}\cdot\hat{\boldsymbol{n}})=\sum_l (Q^l/2^{2l}r^{2(l+1)})\boldsymbol{U}^{(2l)}(\hat{\boldsymbol{r}})\bullet\boldsymbol{U}^{(2l)}(\hat{\boldsymbol{n}}). \tag{3.27}$$

For continuous charge distributions the definitions (3.9) and (3.18) are replaced by integrals over the charge distribution $\rho(\boldsymbol{r})$:

$$Q^{(l)}_{\alpha\ldots\nu}=\int \mathrm{d}^4r\,\rho(\boldsymbol{r})r^{2l}U^{(2l)}_{\alpha\ldots\nu}(\hat{\boldsymbol{r}}), \tag{3.28}$$

where $\mathrm{d}^4r=\Pi^4_{\alpha=1}\,\mathrm{d}r_\alpha$, and

$$Q^l_{mn}=\int \tfrac{1}{8}r^3\,\mathrm{d}r\,\mathrm{d}\Omega\,\rho(\boldsymbol{r})r^{2l}D^l_{mn}(\Omega), \tag{3.29}$$

where $\mathrm{d}\Omega=\mathrm{d}\phi\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\chi$ and the ranges of integration over ϕ, θ and χ are as given in (2.3). In the axially symmetric case, (3.24) becomes

$$Q^l=\frac{4\pi}{2l+1}\int_0^\infty r^3\,\mathrm{d}r\int_0^{2\pi}\tfrac{1}{2}\,\mathrm{d}\psi\,\sin^2\tfrac{1}{2}\psi\rho(r,\psi)r^{2l}U_{2l}(\cos\tfrac{1}{2}\psi) \tag{3.30}$$

(cf e.g. Biedenharn and Louck 1981).

4. Multipole expansion of the energy of a charge distribution in an external field

Suppose now we have a system of charges q_i, $i=1,2,\ldots,N$, in interaction with some specified external potential $\phi(\boldsymbol{r})$, which varies in a smooth, but otherwise arbitrary, manner over the charge distribution. The interaction energy is

$$u=\sum_{i=1}^N q_i\phi(\boldsymbol{r}_i). \tag{4.1}$$

Expanding $\phi(\boldsymbol{r}_i)$ about its value at some origin O chosen within the distribution and using the moment definition (3.9), we find that

$$u=\sum_l [2^{2l}(2l)!]^{-1}(\boldsymbol{\nabla}^{2l}\phi)_0\bullet\boldsymbol{Q}^{(l)}, \tag{4.2}$$

where $\boldsymbol{\nabla}^{2l}=\boldsymbol{\nabla}\boldsymbol{\nabla}\ldots$ ($2l$ factors), and the subscript 0 indicates that the derivatives are to be evaluated at the origin. In deriving (4.2) we have noted that ϕ must obey Laplace's equation, so that the extra terms in $(1/2^{2l})\boldsymbol{Q}^{(l)}$ not contained in $\boldsymbol{M}^{(l)}$ make no contribution to u. Successive terms in (4.2) represent the interaction of the lth-order multipole moment of the charge distribution with the $2l$th derivative of the potential.

In terms of the electric field $\boldsymbol{E}_0 = -(\nabla\phi)_0$, we can write the interaction energy as

$$u = q\phi_0 - \tfrac{1}{2}\boldsymbol{\mu}\cdot\boldsymbol{E}_0 - \tfrac{1}{8}\Theta:(\nabla\boldsymbol{E})_0 - \tfrac{1}{48}\boldsymbol{\Omega}\,\vdots\,(\nabla\nabla\boldsymbol{E})_0 - \tfrac{1}{384}\boldsymbol{\Phi}\,\vdots\,(\nabla\nabla\nabla\boldsymbol{E})_0 - \ldots, \tag{4.3}$$

where $q = Q^{(0)}$, $\boldsymbol{\mu} = \boldsymbol{Q}^{(1/2)}$, $\boldsymbol{\Theta} = \boldsymbol{Q}^{(1)}$, $\boldsymbol{\Omega} = \boldsymbol{Q}^{(3/2)}$, $\boldsymbol{\Phi} = \boldsymbol{Q}^{(2)}$, etc, are the charge, dipole, quadrupole, octopole and hexadecapole moments, etc, of the distribution.

The above equations constitute an expansion of the interaction energy in the spatial derivatives of all orders of the potential. Alternatively, we can expand u as a series in the hyperspherical harmonic expansion coefficients ϕ^l_{mn} of ϕ:

$$\phi(r,\Omega) = \sum_{lmn} \phi^l_{mn} r^{2l} D^l_{mn}(\Omega)^*. \tag{4.4}$$

In (4.4) are included all solutions of $\nabla^2\phi = 0$ which satisfy the assumed boundary condition that ϕ remains finite as $r \to 0$ (cf (2.8)). It follows immediately from (4.1), (4.4) and the definition (3.18) of the moments Q^l_{mn}, that

$$u = \sum_{lmn} \phi^l_{mn} Q^{l*}_{mn}. \tag{4.5}$$

The ϕ^l_{mn} can be related to the hyperspherical components of the gradient of the potential. We define the hyperspherical components ∇_{mn} of ∇ to be

$$\nabla_{1/2\,1/2} = \frac{1}{2}\left(\frac{\partial}{\partial r_4} - \mathrm{i}\frac{\partial}{\partial r_3}\right), \qquad \nabla_{1/2\,-1/2} = -\frac{1}{2}\left(\frac{\partial}{\partial r_2} - \mathrm{i}\frac{\partial}{\partial r_1}\right),$$
$$\nabla_{-1/2\,1/2} = \frac{1}{2}\left(\frac{\partial}{\partial r_2} + \mathrm{i}\frac{\partial}{\partial r_1}\right), \qquad \nabla_{-1/2\,-1/2} = \frac{1}{2}\left(\frac{\partial}{\partial r_4} + \mathrm{i}\frac{\partial}{\partial r_3}\right). \tag{4.6}$$

With this normalisation and choice of phases, we have $\hat{\boldsymbol{r}}\cdot\nabla = \Sigma_{\mu\nu} D^{1/2}_{\mu\nu}(\Omega)^*\nabla_{\mu\nu}$. The Taylor expansion of $\phi(r,\Omega)$ in terms of the ∇_{mn} then reads

$$\phi(r,\Omega) = \sum_l \frac{r^{2l}}{(2l)!}\left(\left(\sum_{\mu\nu} D^{1/2}_{\mu\nu}(\Omega)^*\nabla_{\mu\nu}\right)^{2l}\phi\right)_0. \tag{4.7}$$

Comparing (4.4) with (4.7), we obtain

$$\phi^l_{mn} = \frac{1}{2\pi^2}\frac{(2l+1)}{(2l)!}\int \mathrm{d}\Omega\left(\left(\sum_{\mu\nu} D^{1/2}_{\mu\nu}(\Omega)^*\nabla_{\mu\nu}\right)^{2l}\phi\right)_0 D^l_{mn}(\Omega), \tag{4.8}$$

so that

$$\phi^0_{00} = \phi_0, \qquad \phi^{1/2}_{mn} = (\nabla_{mn}\phi)_0,$$
$$\phi^1_{mn} = \tfrac{1}{2}\sum_{m_1 m_2}\sum_{n_1 n_2} C(\tfrac{1}{2}\tfrac{1}{2}1;\, m_1 m_2 m)C(\tfrac{1}{2}\tfrac{1}{2}1;\, n_1 n_2 n)(\nabla_{m_1 n_1}\nabla_{m_2 n_2}\phi)_0, \tag{4.9}$$

etc. In (4.9) $C(l_1 l_2 l;\, m_1 m_2 m)$ denotes a Clebsch–Gordan coefficient (Rose 1957, Biedenharn and Louck 1981).

5. Multipole expansion of the electrostatic interaction energy of two non-overlapping charge systems

To derive the multipolar expansion of the two-body electrostatic interaction energy

$$u(12)=\sum_{i=1}^{N_1}\sum_{j=1}^{N_2}\frac{q_iq_j}{r_{ij}^2},\tag{5.1}$$

we expand r_{ij}^{-2} as a double Taylor series in $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$ (figure 2):

$$\begin{aligned}r_{ij}^{-2}&=(\boldsymbol{r}-\boldsymbol{r}_i+\boldsymbol{r}_j)^{-2}\\&=\sum_{n_1n_2}\frac{(-)^{n_1}}{n_1!\,n_2!}r_{i\alpha_1}\ldots r_{i\nu_1}r_{j\alpha_2}\ldots r_{j\nu_2}\nabla_{\alpha_1}\ldots\nabla_{\nu_1}\nabla_{\alpha_2}\ldots\nabla_{\nu_2}(1/r^2).\end{aligned}\tag{5.2}$$

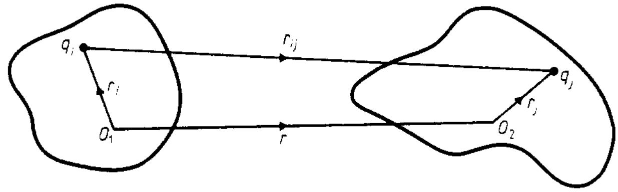

Figure 2. Geometry for the derivation of the multipole expansion, relative to the origins O_1 and O_2, of the electrostatic interaction energy of two non-overlapping charge distributions q_i and q_j.

$\boldsymbol{r}$ is the vector from the origin in system 1 to the origin in system 2. Using the results of § 3, we obtain at once

$$\begin{aligned}u(12)&=\sum_{l_1l_2}\frac{(-)^{2l_2}(2l)!}{(2l_1)!\,(2l_2)!\,r^{2(l+1)}}\boldsymbol{M}^{(l_1)}\bullet\boldsymbol{U}^{(2l)}(\hat{\boldsymbol{r}})\bullet\boldsymbol{M}^{(l_2)}\\&=\sum_{l_1l_2}\frac{(-)^{2l_2}(2l)!}{(2l_1)!\,(2l_2)!\,2^{2l}r^{2(l+1)}}\boldsymbol{Q}^{(l_1)}\bullet\boldsymbol{U}^{(2l)}(\hat{\boldsymbol{r}})\bullet\boldsymbol{Q}^{(l_2)},\end{aligned}\tag{5.3}$$

where $l=l_1+l_2$, and $\boldsymbol{M}^{(l_i)}$ and $\boldsymbol{Q}^{(l_i)}$ are the multipole moments of distribution i ($i=1,2$); $\boldsymbol{Q}^{(l_1)}\bullet\boldsymbol{U}^{(2l)}\bullet\boldsymbol{Q}^{(l_2)}$ denotes the complete contraction $Q^{(l_1)}_{\alpha_1\ldots\nu_1}U^{(2l)}_{\alpha_1\ldots\nu_1,\alpha_2\ldots\nu_2}Q^{(l_2)}_{\alpha_2\ldots\nu_2}$.

For the interaction of two *neutral* charge distributions, the leading terms in $u(12)$ are

$$\begin{aligned}u(12)={}&-\tfrac{1}{2}r^{-4}\boldsymbol{\mu}_1\cdot\boldsymbol{U}^{(2)}\cdot\boldsymbol{\mu}_2+\tfrac{3}{8}r^{-5}\boldsymbol{\mu}_1\cdot\boldsymbol{U}^{(3)}:\boldsymbol{\Theta}_2-\tfrac{3}{8}r^{-5}\boldsymbol{\Theta}_1:\boldsymbol{U}^{(3)}\cdot\boldsymbol{\mu}_2\\&+\tfrac{3}{8}r^{-6}\boldsymbol{\Theta}_1:\boldsymbol{U}^{(4)}:\boldsymbol{\Theta}_2-\tfrac{1}{4}r^{-6}\boldsymbol{\mu}_1\cdot\boldsymbol{U}^{(4)}\,\vdots\,\boldsymbol{\Omega}_2-\tfrac{1}{4}r^{-6}\boldsymbol{\Omega}_1\,\vdots\,\boldsymbol{U}^{(4)}\cdot\boldsymbol{\mu}_2\\&+\tfrac{5}{32}r^{-7}\boldsymbol{\mu}_1\cdot\boldsymbol{U}^{(5)}\,::\,\boldsymbol{\Phi}_2-\tfrac{5}{32}r^{-7}\boldsymbol{\Phi}_1\,::\,\boldsymbol{U}^{(5)}\cdot\boldsymbol{\mu}_2-\tfrac{5}{16}r^{-7}\boldsymbol{\Theta}_1:\boldsymbol{U}^{(5)}\,\vdots\,\boldsymbol{\Omega}_2\\&+\tfrac{5}{16}r^{-7}\boldsymbol{\Omega}_1\,\vdots\,\boldsymbol{U}^{(5)}:\boldsymbol{\Theta}_2+\mathrm{O}(r^{-8}),\end{aligned}\tag{5.4}$$

where $\boldsymbol{\mu}$, $\boldsymbol{\Theta}$, $\boldsymbol{\Omega}$ and $\boldsymbol{\Phi}$ denote $\boldsymbol{Q}^{(l)}$ for $l=\frac{1}{2}$, 1, $\frac{3}{2}$ and 2, respectively. The terms in (5.4) represent the dipole–dipole, dipole–quadrupole, quadrupole–dipole, quadrupole–quadrupole, dipole–octopole, octopole–dipole, dipole–hexadecapole, hexadecapole–dipole, quadrupole–octopole and octopole–quadrupole interaction energies.

Equation (5.3) (and (5.17) below) can also be derived by combining the results of §§ 3 and 4, but the above derivation is more direct.

We next show how $u(12)$ can be expressed in hyperspherical tensor form, using symmetry and electrostatic arguments analogous to the 3D case (Gray 1968, 1976).

First, consider that it must be possible to expand $r_{ij}^{-2}=(\boldsymbol{r}-\boldsymbol{r}_i+\boldsymbol{r}_j)^{-2}$ as a series in the triple products $D^{l_1}_{m_1n_1}(\Omega_i)D^{l_2}_{m_2n_2}(\Omega_j)D^{l}_{mn}(\Omega)^*$, since this function is periodic over the interval 4π in each of the sets of variables Ω_i, Ω_j and Ω:

$$r_{ij}^{-2}=\sum_{l_1l_2l}\sum_{m_1m_2m}\sum_{n_1n_2n}A^{l_1l_2l}_{m_1m_2m,n_1n_2n}(r_ir_jr)D^{l_1}_{m_1n_1}(\Omega_i)D^{l_2}_{m_2n_2}(\Omega_j)D^{l}_{mn}(\Omega)^*, \tag{5.5}$$

where $A^{l_1l_2l}_{m_1m_2m,n_1n_2n}$ is some function of r_i, r_j and r alone.

Second, we observe that the LHS of (5.5) is a scalar, and must therefore be invariant under arbitrary rotations. Using the rotational transformation property (A3.17), we can show that the unique (to within a factor) rotationally invariant combination of products of three hyperspherical harmonics $D^{l_1}_{m_1n_1}(\Omega_i)$, $D^{l_2}_{m_2n_2}(\Omega_j)$ and $D^{l}_{mn}(\Omega)$ is

$$\sum_{m_1m_2m}\sum_{n_1n_2n}C(l_1l_2l;\ m_1m_2m)C(l_1l_2l;\ n_1n_2n)D^{l_1}_{m_1n_1}(\Omega_i)D^{l_2}_{m_2n_2}(\Omega_j)D^{l}_{mn}(\Omega)^* \tag{5.6}$$

(i.e. a generalisation of the usual Clebsch–Gordan series, in which $\Omega_i=\Omega_j=\Omega$); therefore we must have

$$A^{l_1l_2l}_{m_1m_2m,n_1n_2n}(r_ir_jr)=A^{l_1l_2l}(r_ir_jr)C(l_1l_2l;\ m_1m_2m)C(l_1l_2l;\ n_1n_2n), \tag{5.7}$$

where $A^{l_1l_2l}$ is a factor independent of the m's and n's. The properties of the Clebsch–Gordan coefficients (Rose 1957, Biedenharn and Louck 1981) imply a restriction in the summation over indices in (5.5) to $m=m_1+m_2$, $n=n_1+n_2$, and a triangle condition for the l's,

$$l_1+l_2\geqslant l\geqslant|l_1-l_2|. \tag{5.8}$$

Third, we note that r_{ij}^{-2} must satisfy Laplace's equation in each of the variables $\boldsymbol{r}_i$, $\boldsymbol{r}_j$ and $\boldsymbol{r}$, and also the boundary conditions

$$\begin{aligned} r_{ij}^{-2}&\not\to\infty &&\text{as } r_i \text{ or } r_j\to 0,\\ r_{ij}^{-2}&\to 0 &&\text{as } r\to\infty. \end{aligned} \tag{5.9}$$

With the boundary conditions (5.9) we obtain a solution valid in the region of space $r>r_i+r_j$, corresponding to the case where the two charge distributions do not overlap. It follows from (2.8) that

$$A^{l_1l_2l}(r_ir_jr)=A^{l_1l_2l}(r_i^{2l_1}r_j^{2l_2}/r^{2(l+1)}), \tag{5.10}$$

where $A^{l_1l_2l}$ is independent of the r's. To balance the dimensionality of the two sides of (5.5) we must have

$$l=l_1+l_2, \tag{5.11}$$

which is a stronger restriction on the l's than (5.8). The fact that only the maximum value of l occurs is a consequence of the implicitly assumed rigidity of the two charge distributions; for polarisable systems smaller values of l are permitted. Similar results are found in 3D (Gray and van Kranendonk 1966, Gray 1976, Gray and Gubbins 1983).

Finally, the dimensionless constant of proportionality in (5.10) can be obtained by considering some special geometry, e.g. when $\boldsymbol{r}_i$, $\boldsymbol{r}_j$ and $\boldsymbol{r}$ are all parallel. Noting that $D^{l}_{mn}(0)=\delta_{mn}$, and also that

$$\sum_{m_1m_2}C(l_1l_2l;\ m_1m_2m)^2=1 \tag{5.12}$$

(Biedenharn and Louck 1981), we obtain

$$(r-r_i+r_j)^{-2}=\sum_{l_1 l_2}(2l+1)A^{l_1 l_2 l}r_i^{2l_1}r_j^{2l_2}/r^{2(l+1)}. \tag{5.13}$$

Direct expansion of the LHS of (5.13) yields

$$\frac{1}{(r-r_i+r_j)^2}=\sum_{l_1 l_2}(-)^{2l_2}\frac{(2l+1)!}{(2l_1)!(2l_2)!}\frac{r_i^{2l_1}r_j^{2l_2}}{r^{2(l+1)}}, \tag{5.14}$$

and therefore

$$A^{l_1 l_2 l}=(-)^{2l_2}(2l)!/(2l_1)!(2l_2)!. \tag{5.15}$$

The interaction energy $u(12)$ is consequently found to be

$$u(12)=\sum_{l_1 l_2}\sum_{m_1' m_2'}\sum_{n_1 n_2}\frac{(-)^{2l_2}(2l)!}{(2l_1)!(2l_2)!\,r^{2(l+1)}}\times C(l_1 l_2 l;\, m_1 m_2 m)C(l_1 l_2 l;\, n_1 n_2 n)Q^{l_1}_{m_1 n_1}Q^{l_2}_{m_2 n_2}D^{l}_{mn}(\Omega)^*. \tag{5.16}$$

Here $Q^{l_1}_{m_1 n_1}$ and $Q^{l_2}_{m_2 n_2}$ are space-fixed components for distributions 1 and 2 respectively. $u(12)$ can be written instead in a form involving the components $Q^{l_1}_{m_1' n_1'}$ and $Q^{l_2}_{m_2' n_2'}$ defined in frames rigidly attached to the two bodies of charge, and which shows explicitly the orientational dependences, using the rotational transformation property (A3.18) of the moments derived in appendix 3. We find

$$\begin{aligned}u(12)=\sum_{l_1 l_2}\sum_{m_1 m_2}\sum_{n_1 n_2}\sum_{m_1' m_2'}\sum_{n_1' n_2'}&\frac{(-)^{2l_2}(2l)!}{(2l_1)!(2l_2)!\,r^{2(l+1)}}Q^{l_1}_{m_1' n_1'}Q^{l_2}_{m_2' n_2'}\\ &\times C(l_1 l_2 l;\, m_1 m_2 m)C(l_1 l_2 l;\, n_1 n_2 n)\\ &\times D^{l_1}_{m_1 m_1'}(\Omega_1)D^{l_1}_{n_1' n_1}(\tilde{\Omega}_1)D^{l_2}_{m_2 m_2'}(\Omega_2)D^{l_2}_{n_2' n_2}(\tilde{\Omega}_2)D^{l}_{mn}(\Omega)^*.\end{aligned} \tag{5.17}$$

Here $(\Omega_i, \tilde{\Omega}_i)$ are the Euler angles specifying the orientation of the body-fixed frame of distribution i ($i=1,2$) relative to the space-fixed frame (in 4D the relative orientation of two axis systems is in general specified by *six* angles).

If both charge distributions are axially symmetric, (5.17) simplifies to

$$\begin{aligned}u(12)=\sum_{l_1 l_2}\sum_{m_1 m_2}\sum_{n_1 n_2}&\frac{(-)^{2l_2}(2l)!}{(2l_1)!(2l_2)!\,r^{2(l+1)}}Q^{l_1}Q^{l_2}\\ &\times C(l_1 l_2 l;\, m_1 m_2 m)C(l_1 l_2 l;\, n_1 n_2 n)D^{l_1}_{m_1 n_1}(\Omega_1)D^{l_2}_{m_2 n_2}(\Omega_2)D^{l}_{mn}(\Omega)^*.\end{aligned} \tag{5.18}$$

In (5.18), Q^{l_i} is the unique multipole moment of order l_i for the distribution i, and Ω_i specifies the orientation of the symmetry axis of distribution i ($i=1,2$) relative to the space-fixed frame. Equation (5.18) also follows from (5.16) and (3.23).

The Cartesian analogue of (5.18) is

$$u(12)=\sum_{l_1 l_2}\frac{(-)^{2l_2}(2l)!}{(2l_1)!(2l_2)!\,2^{2l}r^{2(l+1)}}Q^{l_1}Q^{l_2}U^{(2l_1)}(\hat{\boldsymbol{n}}_1)\bullet U^{(2l)}(\hat{\boldsymbol{r}})\bullet U^{(2l_2)}(\hat{\boldsymbol{n}}_2), \tag{5.19}$$

as deduced from (5.3) and (3.26). In (5.19) $\hat{\boldsymbol{n}}_i$ is a unit vector along the direction of the symmetry axis of distribution i ($i=1,2$).

Using (5.19) together with (A2.4) we can write the explicit expressions for the energies of interaction between two dipoles ($u_{1/21/21}$) and between two axial quadrupoles (u_{112}) as

$$u_{1/21/21} = \tfrac{1}{2}r^{-4}\mu_1\mu_2(\cos\tfrac{1}{2}\psi_{12} - 4\cos\tfrac{1}{2}\psi_1\cos\tfrac{1}{2}\psi_2) \tag{5.20}$$

and

$$u_{112} = \tfrac{2}{3}r^{-6}\Theta_1\Theta_2(16\cos^2\tfrac{1}{2}\psi_1\cos^2\tfrac{1}{2}\psi_2 - 8\cos\tfrac{1}{2}\psi_1\cos\tfrac{1}{2}\psi_{12}\cos\tfrac{1}{2}\psi_2 - 2\cos^2\tfrac{1}{2}\psi_1 - 2\cos^2\tfrac{1}{2}\psi_2 + \tfrac{2}{3}\cos^2\tfrac{1}{2}\psi_{12} + \tfrac{1}{3}), \tag{5.21}$$

where μ_i and Θ_i are the Cartesian components $\mu_{4'}$ and $\Theta_{4'4'}$, respectively, if the body-fixed $4'$ axes are chosen coincident with $\hat{\boldsymbol{n}}_i$, $\cos\frac{1}{2}\psi_i = \hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{r}}$ $(i=1,2)$ and $\cos\frac{1}{2}\psi_{12} = \hat{\boldsymbol{n}}_1\cdot\hat{\boldsymbol{n}}_2$.

Joslin and Gray (1983) showed that in *two* dimensions the interaction energy of a given pair of multipoles is somewhat unusual in that there is an infinity of minima (preferred relative orientations). As these authors pointed out, this probably implies that much of the physics of 2D multipolar fluids and lattices differs fundamentally from that of their 3D analogues. In 4D, however, the situation appears to be qualitatively similar to the 3D case. For example, we can see from (5.20) that there are only two minimum-energy configurations for two interacting dipoles, the familiar head-to-tail arrangements $\hat{\boldsymbol{\mu}}_1\cdot\hat{\boldsymbol{r}} = \hat{\boldsymbol{\mu}}_2\cdot\hat{\boldsymbol{r}} = \pm 1$. Similarly, from (5.21) there are only four minima for two interacting identical, axially symmetric quadrupoles, the 'T'-shaped conformations $\hat{\boldsymbol{n}}_1\cdot\hat{\boldsymbol{r}} = \pm 1$, $\hat{\boldsymbol{n}}_2\cdot\hat{\boldsymbol{r}} = 0$ and $\hat{\boldsymbol{n}}_1\cdot\hat{\boldsymbol{r}} = 0$, $\hat{\boldsymbol{n}}_2\cdot\hat{\boldsymbol{r}} = \pm 1$.

6. Convergence of the expansions

We can readily establish that the multipole expansion of the potential of § 3 converges for all points outside the charge distribution, i.e. provided $r > r_i$, $i = 1, 2, \ldots, N$. Similarly, the expansion of the two-body interaction energy of § 5 is convergent if the two charge distributions do not overlap. However, in the event that one deals not with discrete distributions of charge, but rather with some specified charge density $\rho(\boldsymbol{r})$ which does not vanish exactly outside some region of space, convergence may only be asymptotic, as in 3D (Jansen 1958).

Acknowledgment

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Appendix 1. The number of independent components of the multipole moment of order l (rank $2l$)

The Cartesian moments $\boldsymbol{M}^{(l)}$ and $\boldsymbol{Q}^{(l)}$ each have 4^{2l} components $M^{(l)}_{\alpha\ldots\nu}$ and $Q^{(l)}_{\alpha\ldots\nu}$ without regard to symmetry under permutation of the indices. When this symmetry is taken into consideration the number of independent components of $\boldsymbol{M}^{(l)}$ drops to

$$N_l = \sum_{n_1=0}^{2l}\sum_{n_2=0}^{2l-n_1}\sum_{n_3=0}^{2l-n_1-n_2} 1, \tag{A1.1}$$

since of the $2l$ indices $0 \leqslant n_1 \leqslant 2l$ can be 1, $0 \leqslant n_2 \leqslant 2l - n_1$ can be 2, $0 \leqslant n_3 \leqslant 2l - n_1 - n_2$ can be 3, and the remainder must be 4. Straightforward evaluation of the sums in (A1.1) yields

$$N_l = \tfrac{1}{6}(2l+1)(2l+2)(2l+3). \tag{A1.2}$$

The tracelessness of the $\boldsymbol{Q}^{(l)}$ further reduces the number of independent components of this tensor below those of $\boldsymbol{M}^{(l)}$: $Q^{(l)}_{\alpha\alpha,\gamma\ldots\nu} = 0$ makes N_{l-2} independent restrictions on the $Q^{(l)}_{\alpha\ldots\nu}$. Thus there are at most $N_l - N_{l-2} = (2l+1)^2$ independent components of $\boldsymbol{Q}^{(l)}$.

This result is consistent with the definition of the hyperspherical tensor moments Q^l_{mn} in terms of the harmonics D^l_{mn} (equation (3.18)), since m and n can each assume $2l+1$ values ($|m| \leqslant l$, $|n| \leqslant l$).

Appendix 2. Relation between the Cartesian and hyperspherical components of the multipole moment tensors

In this appendix we discuss the relation between the Cartesian

$$Q^{(l)}_{\alpha\ldots\nu} = \sum_i q_i r_i^{2l} U^{(2l)}_{\alpha\ldots\nu}(\hat{\boldsymbol{r}}_i) \tag{A2.1}$$

and hyperspherical

$$Q^l_{mn} = \sum_i q_i r_i^{2l} D^l_{mn}(\Omega_i) \tag{A2.2}$$

components of the multipole moment tensors.

In the absence of any symmetry in the distribution of charge, the relationship between the two forms (A2.1) and (A2.2) is a complicated one. We note that even in 3D the completely general result has never been derived in a simple, explicit form (see Joslin and Gray (1983) for the 2D case). However, the explicit results for the first few moments are easily written down by expressing the hyperspherical harmonics $D^l_{mn}(\Omega)$ in terms of the Euler angles (ϕ, θ, χ) (see e.g. Brink and Satchler 1968), thence in terms of (r_1, r_2, r_3, r_4) using (2.2), and finally in terms of $U^{(2l)}_{\alpha\ldots\nu}(\hat{\boldsymbol{r}})$ using the definitions (3.4). In this way we find straightforwardly, using the notation previously introduced to denote the charge, dipole and quadrupole moments:

charge: $Q^0_{00} = q$;

dipole: $Q^{1/2}_{1/2\,1/2} = \tfrac{1}{2}(\mu_2 - \mathrm{i}\mu_3)$, $\quad Q^{1/2}_{1/2\,-1/2} = -\tfrac{1}{2}(\mu_2 - \mathrm{i}\mu_1)$,

$Q^{1/2}_{-1/2\,1/2} = \tfrac{1}{2}(\mu_2 + \mathrm{i}\mu_1)$, $\quad Q^{1/2}_{-1/2\,-1/2} = \tfrac{1}{2}(\mu_4 + \mathrm{i}\mu_3)$;

quadrupole: $Q^1_{11} = \tfrac{1}{4}(\Theta_{44} - 2\mathrm{i}\Theta_{43} - \Theta_{33})$, $\quad Q^1_{-1-1} = \tfrac{1}{4}(\Theta_{44} + 2\mathrm{i}\Theta_{43} - \Theta_{33})$,

$Q^1_{1-1} = \tfrac{1}{4}(\Theta_{22} - 2\mathrm{i}\Theta_{21} - \Theta_{11})$, $\quad Q^1_{-11} = \tfrac{1}{4}(\Theta_{22} + 2\mathrm{i}\Theta_{21} - \Theta_{11})$,

$Q^1_{00} = \tfrac{1}{4}(\Theta_{44} + \Theta_{33} - \Theta_{22} - \Theta_{11})$, $\quad Q^1_{10} = -\tfrac{1}{4}\sqrt{2}(\Theta_{42} - \mathrm{i}\Theta_{32} - \mathrm{i}\Theta_{41} - \Theta_{31})$,

$Q^1_{-10} = \tfrac{1}{4}\sqrt{2}(\Theta_{42} + \mathrm{i}\Theta_{32} + \Theta_{41} - \Theta_{31})$, $\quad Q^1_{01} = \tfrac{1}{4}\sqrt{2}(\Theta_{42} - \mathrm{i}\Theta_{32} + \mathrm{i}\Theta_{41} + \Theta_{31})$,

$Q^1_{0-1} = -\tfrac{1}{4}\sqrt{2}(\Theta_{42} + \mathrm{i}\Theta_{32} - \mathrm{i}\Theta_{41} + \Theta_{31})$. (A2.3)

In the *axially-symmetric* case a simple relation exists between the unique Cartesian and hyperspherical multipole moments in all orders l. If we set up a body-fixed coordinate axis system S' such that the 4'-axis is coincident with the symmetry axis $\hat{\boldsymbol{n}}$, then $\boldsymbol{Q}^{(l)} \bullet \hat{\boldsymbol{n}}^{2l} = Q^{(l)}_{4'\ldots4'}$, and (A3.21) becomes

$$Q^l = \frac{1}{2l+1} Q^{(l)}_{4'\ldots4'}. \tag{A2.4}$$

Appendix 3. Transformation properties of the multipole moments under translations, rotations and reflections

In this appendix we derive the transformation properties of the multipole moments under (a) translation of the coordinate axis system (§ A3.1), and (b) the symmetry operations of the 4D rotation–reflection group O_4 (§ A3.2). The general results are presented for the hyperspherical tensor moments Q^l_{mn}, because they are more simply derived than the corresponding results for the Cartesian moments $Q^{(l)}_{\alpha\ldots\nu}$.

A3.1. Translation of the coordinate axis system

Consider two frames S and S' in arbitrary relative translation. The origin O' of S' is displaced by $\boldsymbol{a}$ from the origin O of S. The coordinates of a point P are represented by the vector $\boldsymbol{r}$ in S and by $\boldsymbol{r}' = \boldsymbol{r} - \boldsymbol{a}$ in S'. In S' we measure a multipole moment $Q'^{l'}_{m'n'}$ (or $Q^{l'}_{m'n'}$ for brevity) given by

$$Q^{l'}_{m'n'} = \sum_i q_i r_i'^{2l'} D^{l'}_{m'n'}(\Omega_i'), \tag{A3.1}$$

which we seek to relate to the moments

$$Q^l_{mn} = \sum_i q_i r_i^{2l} D^l_{mn}(\Omega_i) \tag{A3.2}$$

measured in S. The procedure we employ is analogous to that adopted by Gray (1976) in 3D (see also Gray and Gubbins (1983)).

We introduce the notation

$$f^{l'}_{m'n'}(\boldsymbol{r}, \boldsymbol{a}) = r'^{2l'} D^{l'}_{m'n'}(\Omega'). \tag{A3.3}$$

We expand $f^{l'}_{m'n'}(\boldsymbol{r}, \boldsymbol{a})$ in terms of the hyperspherical harmonics of the orientations Ω of $\boldsymbol{r}$ and $\Omega_{\hat{a}}$ of $\boldsymbol{a}$. In order that this quantity transform properly under rotations of the coordinate axis system, i.e. like a hyperspherical tensor of rank $2l'$, the expansion must take the form

$$f^{l'}_{m'n'}(\boldsymbol{r}, \boldsymbol{a}) = \sum_{ll_2} \sum_{mm_2} \sum_{nn_2} f^{ll_2l'}(r, a) C(ll_2l'; mm_2m') C(ll_2l'; nn_2n') D^l_{mn}(\Omega) D^{l_2}_{m_2n_2}(\Omega_{\hat{a}}). \tag{A3.4}$$

(The proof of (A3.4) follows closely along the lines of the argument which establishes (5.6) as the unique rotationally invariant combination of products of three hyperspherical harmonics.) Here $f^{ll_2l'}(r, a)$ is a function of r and a alone. Since $f^{l'}_{m'n'}(\boldsymbol{r}, \boldsymbol{a})$ is a solution of Laplace's equation in $\boldsymbol{r}'$, it must also be a solution in $\boldsymbol{r}$ and $\boldsymbol{a}$. Therefore we have

$$f^{ll_2l'}(r, a) = f^{ll_2l'} r^{2l} a^{2l_2}, \tag{A3.5}$$

where $f^{ll_2l'}$ is independent of r and a. We allow only those solutions which satisfy the boundary condition that $f^{l'}_{m'n'}(\boldsymbol{r}, \boldsymbol{a})$ remain finite as $r \to 0$ or $a \to 0$. Dimensional considerations imply that in (A3.5) and successive equations, $l + l_2 = l'$.

To evaluate the dimensionless constant of proportionality in (A3.5) we can consider the special geometry $\Omega = \Omega_{\hat{a}} = \Omega' = 0$. Since $D^l_{mn}(0) = \delta_{mn}$, and using (5.12), we find

$$(r-a)^{2l'} = \sum_{ll_2} f^{ll_2l'} r^{2l} a^{2l_2}, \tag{A3.6}$$

whence

$$f^{ll_2l'} = (-)^{2l_2}(2l')!/(2l)!(2l_2)!. \tag{A3.7}$$

Therefore we find

$$Q^{l'}_{m'n'} = \sum_{ll_2} \sum_{mm_2} \sum_{nn_2} \frac{(-)^{2l_2}(2l')!}{(2l)!(2l_2)!} C(ll_2l';\, mm_2m')C(ll_2l';\, nn_2n')Q^l_{mn} a^{2l_2} D^{l_2}_{\bar{m}_2n_2}(\Omega_{\hat{a}}). \tag{A3.8}$$

Note that the coefficient of $Q^{l'}_{mn}$ on the RHS of (A3.8) is $\delta_{mm'}\delta_{nn'}$. The change in the multipole moment of order l' on passing from S to S' involves the lower order moments $l = l' - \frac{1}{2},\ l' - 1, \ldots, 0$. The first non-vanishing moment, in particular, is origin independent.

For the first few Cartesian moments we find

$$q' = q, \qquad \boldsymbol{\mu}' = \boldsymbol{\mu} - 2q\boldsymbol{a},$$
$$\boldsymbol{\Theta}' = \boldsymbol{\Theta} - 2\boldsymbol{\mu}\boldsymbol{a} - 2\boldsymbol{a}\boldsymbol{\mu} + (\boldsymbol{\mu}\cdot\boldsymbol{a})\mathbf{1} + q(4\boldsymbol{a}\boldsymbol{a} - a^2\mathbf{1}). \tag{A3.9}$$

In the axially symmetric case, translating the origin a distance a along the symmetry axis transforms the scalar moment (3.24) into

$$Q^{l'} = \sum_{ll_2} \frac{(-)^{2l_2}(2l')!}{(2l)!(2l_2)!} a^{2l_2} Q^l. \tag{A3.10}$$

A3.2. The symmetry operations of the 4D rotation–reflection group O_4

All possible symmetry operations of the orthogonal group O_4 (all operations which leave unchanged the quadratic form $\Sigma^4_{\alpha=1} r^2_\alpha$) can be generated from the appropriate combination of just two operations: (i) a suitably general proper rotation of the coordinate axis system, and (ii) an improper rotation, or reflection.

(i) *Rotation of the coordinate axis system*

In 4D the relative orientation of two axis systems is in general specified by six angles, or, alternatively, by two sets of quaternion parameters, (r_1, r_2, r_3, r_4) and $(\tilde{r}_1, \tilde{r}_2, \tilde{r}_3, \tilde{r}_4)$, which are defined in terms of $\Omega = (\phi, \theta, \chi)$ and $\tilde{\Omega} = (\tilde{\phi}, \tilde{\theta}, \tilde{\chi})$ analogously to (2.2) (with $r = 1$).

Under the passive rotation Ω, the coordinates of a point $\boldsymbol{R} = (R_1, R_2, R_3, R_4)$ are transformed to $\boldsymbol{R}' = (R'_1, R'_2, R'_3, R'_4)$ such that

$$\begin{pmatrix} R'_1 \\ R'_2 \\ R'_3 \\ R'_4 \end{pmatrix} = \begin{pmatrix} r_4 & r_3 & -r_2 & r_1 \\ -r_3 & r_4 & r_1 & r_2 \\ r_2 & -r_1 & r_4 & r_3 \\ -r_1 & -r_2 & -r_3 & r_4 \end{pmatrix} \begin{pmatrix} R_1 \\ R_2 \\ R_3 \\ R_4 \end{pmatrix} \tag{A3.11}$$

(Casimir 1931). Note that as a three-parameter transformation, Ω cannot in itself accomplish the most general rotation of the axes. Thus, the matrix of the r_α's in (A3.11) is reducible (in the complex basis of the Cayley–Klein parameters):

$$\begin{pmatrix} R_4'-\mathrm{i}R_3' \\ R_2'+\mathrm{i}R_1' \\ -(R_2'-\mathrm{i}R_1') \\ R_4'+\mathrm{i}R_3' \end{pmatrix} = \begin{pmatrix} \boldsymbol{M} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{M} \end{pmatrix} \begin{pmatrix} R_4-\mathrm{i}R_3 \\ R_2+\mathrm{i}R_1 \\ -(R_2-\mathrm{i}R_1) \\ R_4+\mathrm{i}R_3 \end{pmatrix}, \tag{A3.12}$$

where $\boldsymbol{0}$ is the 2×2 null matrix, and

$$\boldsymbol{M} = \begin{pmatrix} r_4-\mathrm{i}r_3 & -(r_2-\mathrm{i}r_1) \\ r_2+\mathrm{i}r_1 & r_4+\mathrm{i}r_3 \end{pmatrix}; \tag{A3.13}$$

we recognise $\boldsymbol{M}$ as the transformation matrix $D^{1/2}(\Omega)$. Hence Ω mixes only the pairs $R_4\mp\mathrm{i}R_3\leftrightarrow\pm(R_2\pm\mathrm{i}R_1)$. To effect the mixing $R_4\mp\mathrm{i}R_3\leftrightarrow\mp(R_2\mp\mathrm{i}R_1)$ we apply a second rotation $\tilde{\Omega}$ such that

$$\begin{pmatrix} R_1'' \\ R_2'' \\ R_3'' \\ R_4'' \end{pmatrix} = \begin{pmatrix} \tilde{r}_4 & -\tilde{r}_3 & \tilde{r}_2 & \tilde{r}_1 \\ \tilde{r}_3 & \tilde{r}_4 & -\tilde{r}_1 & \tilde{r}_2 \\ -\tilde{r}_2 & \tilde{r}_1 & \tilde{r}_4 & \tilde{r}_3 \\ -\tilde{r}_1 & -\tilde{r}_2 & -\tilde{r}_3 & \tilde{r}_4 \end{pmatrix} \begin{pmatrix} R_1' \\ R_2' \\ R_3' \\ R_4' \end{pmatrix}, \tag{A3.14}$$

or equivalently

$$\begin{pmatrix} R_4''-\mathrm{i}R_3'' \\ -(R_2''-\mathrm{i}R_1'') \\ R_2''+\mathrm{i}R_1'' \\ R_4''+\mathrm{i}R_3'' \end{pmatrix} = \begin{pmatrix} \tilde{\boldsymbol{M}}^{\mathrm{T}} & \boldsymbol{0} \\ \boldsymbol{0} & \tilde{\boldsymbol{M}}^{\mathrm{T}} \end{pmatrix} \begin{pmatrix} R_4'-\mathrm{i}R_3' \\ -(R_2'-\mathrm{i}R_1') \\ R_2'+\mathrm{i}R_1' \\ R_4'+\mathrm{i}R_3' \end{pmatrix}, \tag{A3.15}$$

where $\tilde{\boldsymbol{M}}^{\mathrm{T}}$ is the transpose of a matrix $\tilde{\boldsymbol{M}}$ defined analogously to (A3.13), but with $\tilde{r}_\alpha$ replacing r_α.

It is obvious that with successive application of the (commuting) operations Ω and $\tilde{\Omega}$, we can accomplish any coordinate transformation with determinant $=+1$, i.e. a general proper rotation of the coordinate axis system.

We can combine (A3.12) and (A3.15) and write the result in the compact form

$$D^{1/2}_{m''n''}(\Omega_{\boldsymbol{R}''}) = \sum_{mn} D^{1/2}_{m''m}(\Omega) D^{1/2}_{mn}(\Omega_{\boldsymbol{R}}) D^{1/2}_{nn''}(\tilde{\Omega}). \tag{A3.16}$$

It can then be shown that under the combined effect of Ω and $\tilde{\Omega}$, for any l, the hyperspherical harmonics $D^l_{mn}(\Omega_{\boldsymbol{R}})$ transform according to

$$D^l_{m''n''}(\Omega_{\boldsymbol{R}''}) = \sum_{mn} D^l_{m''m}(\Omega) D^l_{mn}(\Omega_{\boldsymbol{R}}) D^l_{nn''}(\tilde{\Omega}). \tag{A3.17}$$

Note that the effect of Ω on $D^l_{mn}(\Omega_{\boldsymbol{R}})$ is to scramble the index m, leaving n unchanged, while $\tilde{\Omega}$ has exactly the opposite effect. The form of (A3.17) is associated with the homomorphism of O_4 to the direct product $SU_2\otimes SU_2$ (Biedenharn 1961, Talman 1968).

It follows immediately from (A3.17) and the definition (3.18) that under the proper rotation $(\Omega, \tilde{\Omega})$, the hyperspherical tensor multipole moments Q^l_{mn} transform according to

$$Q^l_{m''n''} = \sum_{mn} D^l_{m''m}(\Omega) Q^l_{mn} D^l_{nn''}(\tilde{\Omega}). \tag{A3.18}$$

For an *axially symmetric* distribution of charge, Q^l_{mn} depends only on $\Omega_{\hat{n}}$, the set of Euler angles specifying the direction of the symmetry axis $\hat{\boldsymbol{n}}$ in four-space, and its transformation properties must be those of the hyperspherical harmonic $D^l_{mn}(\Omega_{\hat{n}})$ (see Joslin and Gray (1983) and Gray (1968 or 1976) or Gray and Gubbins (1983) for the corresponding results in 2D and 3D). Thus we have

$$Q^l_{mn} = Q^l D^l_{mn}(\Omega_{\hat{n}}), \tag{A3.19}$$

where the constant of proportionality is identified as the unique multipole moment of order l in the principal axis system $\Omega_{\hat{n}} = 0$: i.e. Q^l = any diagonal body-fixed element $Q^l_{m'm'}$.

The Cartesian analogue of (A3.19) is

$$Q^{(l)}_{\alpha\ldots\nu} = Q^l U^{(2l)}_{\alpha\ldots\nu}(\hat{\boldsymbol{n}}). \tag{A3.20}$$

To prove (A3.20) we simply note that when there is axial symmetry, the moment $\boldsymbol{Q}^{(l)}$ can depend only on $\hat{\boldsymbol{n}}$; and that, to within a factor, $\boldsymbol{U}^{(2l)}(\hat{\boldsymbol{n}})$ is the unique symmetric, traceless, $2l$th-rank tensor function of $\hat{\boldsymbol{n}}$. To show that the proportionality constant in (A3.20) is indeed Q^l it is then only necessary to note that forming the full contraction of $\boldsymbol{Q}^{(l)}$ with $\hat{\boldsymbol{n}}^{2l}$ yields

$$Q^l = (2l+1)^{-1}\boldsymbol{Q}^{(l)} \bullet \hat{\boldsymbol{n}}^{2l}, \tag{A3.21}$$

which is consistent with (3.9) and (3.24).

Note that in 4D the inversion operation $(R_1, R_2, R_3, R_4) \to (-R_1, -R_2, -R_3, -R_4)$ has determinant = +1, and can therefore be accomplished by a proper rotation of the coordinate axis system; this is not of course the case in 3D, but also holds in 2D, or indeed in any space of even dimensionality. Inversion is effected by changing any of ϕ, θ or χ by 2π, and it follows that the moments transform as

$$Q^l_{mn} \to Q^l_{m'n'} = (-)^{2l} Q^l_{mn}. \tag{A3.22}$$

(ii) *Reflection in the $R_1R_2R_3$ subspace*
The reflection

$$(R_1, R_2, R_3, R_4) \to (R_1, R_2, R_3, -R_4) \tag{A3.23}$$

is a symmetry operation with determinant = −1. This improper rotation is accomplished by the Euler angle transformation

$$(\phi, \theta, \chi) \to (-\chi + \pi, \theta + 2\pi, -\phi - \pi). \tag{A3.24}$$

Using (3.18) and the known properties of the $D^l_{mn}(\Omega)$ (Brink and Satchler 1968), we find for the transformed moment

$$Q^l_{m'n'} = (-)^{2l+m-n} Q^l_{-n-m}. \tag{A3.25}$$

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