Bipolar Expansion of Coulombic Potentials*

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The calculation classically or quantum mechanically of the coulombic interaction between two charge distributions is greatly simplified by use of the bipolar expansion:

$$\frac{1}{r_{12}}=\sum_{n_1,n_2,m} B_{n_1,n_2}{}^{|m|}(r_1,r_2;R)P_{n_1}{}^{|m|}(\cos\theta_1)P_{n_2}{}^{|m|}(\cos\theta_2)\exp[im(\phi_2-\phi_1)].$$

Here (r_1, θ_1, ϕ_1) are the spherical coordinates at a point referred to the center of the first charge distribution, and (r_2, θ_2, ϕ_2) are the spherical coordinates of another point referred to the center of the second distribution; R is the separation between the centers; r_{12} is the distance between the two points; $P_n{}^{|m|}(\cos\theta)$ are the associated Legendre polynomials; the $B_{n_1,n_2}{}^{|m|}(r_1,r_2;R)$ are expansion coefficients given in this paper. There are four functional forms for these coefficients, depending on the ratios of r_1, r_2, and R. Three of these have been given recently by Carlson and Rushbrooke. For quantum-mechanical problems involving overlapping charge distributions, the fourth case, $|r_1-r_2|\leqslant R\leqslant r_1+r_2$, must be considered as well. Here the coefficients have a more complicated form. The solution is expressed as an integral, and a number of the coefficients are tabulated. The expansion permits a simple evaluation of the two center coulombic integrals arising in a large variety of quantum-mechanical problems.

THE problem of calculating the coulombic interactions between two charge distributions in either classical or quantum mechanics can often be simplified by using an expansion of $1/r_{12}$ in terms of products of surface harmonics in the two coordinate systems characteristic of the two distributions. Here r_{12} is the distance between a point in distribution 1 and a point in distribution 2. Let a be an origin located in 1; b be an origin in 2; R be the distance between a and b; θ_1 be the internal angle that a radius vector to a point in 1 makes with the line ab; θ_2 be the internal angle that a radius vector to a point in 2 makes with the line ab; let ϕ_1 and ϕ_2 be the angles which the projections of the radius vector make with an axis perpendicular to ab. Figure 1 shows the geometry. The convenient expansion is, then,

$$1/r_{12}=\sum_{n_1,n_2,m} B_{n_1,n_2}{}^{|m|}(r_1,r_2;R)P_{n_1}{}^{|m|}(\cos\theta_1)\times P_{n_2}{}^{|m|}(\cos\theta_2)\exp[im(\phi_2-\phi_1)]. \quad (1)$$

Here n_1 and n_2 go from zero to infinity and m goes from $-n_<$ to $n_<$, where $n_<$ is the lesser of n_1 and n_2. The $P_n{}^m(\cos\theta)$ are the associated Legendre polynomials defined by[1]

$$P_n{}^m(x)=(-1)^m(1-x^2)^{m/2}[d^m/dx^m]P_n(x). \quad (2)$$

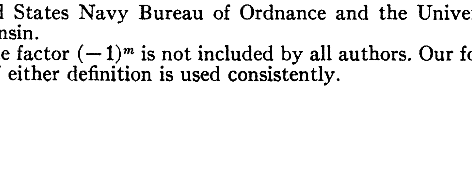

FIG. 1. Coordinates for the bipolar expansion. r_{12} is the distance between points 1 and 2.

Recently Carlson and Rushbrooke[2] have considered this problem. They obtained expressions for $B_{n_1n_2}{}^{|m|}(r_1,r_2;R)$ provided that $R>r_1+r_2$, $r_2>R+r_1$, or $r_1>R+r_2$. The first condition always applies if the charge distributions do not overlap. However, for overlapping charge distributions such as occur in quantum-mechanical problems it is also necessary to consider another region, $|r_1-r_2|\leqslant R\leqslant r_1+r_2$, which seems to have escaped the attention of Carlson and Rushbrooke. The expressions for the B's are much more difficult to obtain for this region and are the principal subject of attention in the present paper.

An arbitrary charge distribution, $\rho(1;x_1,y_1,z_1)$, can be expressed as the sum of an infinite series of radial functions times surface harmonics:

$$\rho(1;x_1,y_1,z_1)=\sum_{n_1=0}^{\infty}\sum_{m_1=-n_1}^{n_1}\rho_{n_1m_1}(1;r_1)\times P_{n_1}{}^{|m_1|}(\cos\theta_1)\exp(im_1\phi_1), \quad (3)$$

and a second charge distribution, $\rho(2;x_2,y_2,z_2)$. can be expressed in the form

$$\rho(2;x_2,y_2,z_2)=\sum_{n_2=0}^{\infty}\sum_{m_2=-n_2}^{n_2}\rho_{n_2m_2}(2;r_2)\times P_{n_2}{}^{|m_2|}(\cos\theta_2)\exp(im_2\phi_2). \quad (4)$$

Here ρ_{00} determines the net charge in the distribution; $\rho_{1,-1}$, $\rho_{1,0}$, $\rho_{1,1}$ determine its dipole moment; $\rho_{2,-2}$, $\rho_{2,-1}$, $\rho_{2,0}$, $\rho_{2,1}$, $\rho_{2,2}$ determine its quadrupole moment; etc. The electrostatic energy of interaction between the two charge distributions is

$$V_{12}=\iint[\rho(1;x_1,y_1,z_1)\rho(2;x_2,y_2,z_2)/r_{12}]d\tau_1d\tau_2. \quad (5)$$

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[1] The factor $(-1)^m$ is not included by all authors. Our formulas hold if either definition is used consistently.

[2] B. C. Carlson and G. S. Rushbrooke, Proc. Cambridge Phil. Soc. 46, 626 (1950).

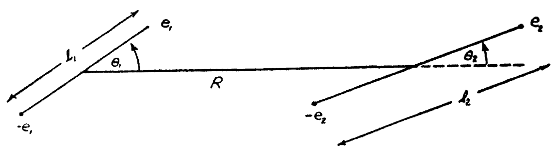

FIG. 2. Interacting dipoles.

Substituting Eqs. (1), (3), and (4) into Eq. (5) and making use of the orthogonality relations between the spherical harmonics, it follows after integrating over the angles that

$$V_{12}=\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\sum_{m=-n_<}^{n_<}\frac{16\pi^2}{(2n_1+1)(2n_2+1)}\times\frac{(n_1+|m|)!(n_2+|m|)!}{(n_1-|m|)!(n_2-|m|)!}\cdot\int_0^\infty\int_0^\infty B_{n_1n_2}{}^{|m|}(r_1,r_2;R)\rho_{n_1m}(1;r_1)\times\rho_{n_2m}(2;r_2)r_1^2r_2^2dr_1dr_2. \quad (6)$$

The problem of evaluating V_{12} is thus considerably reduced by the introduction of the bipolar expansion.

The charge distributions are usually expressed with respect to principal axes located within the charge distribution and oriented so as to diagonalize some tensor property of the system. Thus,

$$\rho(1;x_1,y_1,z_1)=\sum_{n_1=0}^{\infty}\sum_{m_1'=-n_1}^{n_1}\rho_{n_1m_1}{}'(1;r_1)\times P_{n_1}{}^{|m_1'|}(\cos\theta_1')\exp(im_1'\phi_1'), \quad (7)$$

where θ_1' and ϕ_1' are the angles that the point in question makes with the principal axes. Similarly, a second charge distribution would be expressed in terms of its principal axes:

$$\rho(2;x_2,y_2,z_2)=\sum_{n_2=0}^{\infty}\sum_{m_2'=-n_2}^{n_2}\rho_{n_2m_2}{}'(2;r_2)\times P_{n_2}{}^{|m_2'|}(\cos\theta_2')\exp(im_2'\phi_2'). \quad (8)$$

But by simple group theory, the radial functions $\rho_{n_1m_1}{}'(1;r_1)$ can be related to the $\rho_{n_1m_1}(1;r_1)$ of the previous example, Eq. (3), and the $\rho_{n_2m_2}{}'(2;r_2)$ can be related to the $\rho_{n_2m_2}(2;r_2)$ of Eq. (4). Let S_1 and S_2 be the rotations which turn the two principal axes systems respectively into coincidence with a fixed laboratory reference frame. Then let T be a rotation which turns the Z axis of the laboratory frame into an orientation parallel to the line passing from the origin of the first distribution to the origin of the second. Then TS_1 and TS_2 respectively turn the principal axes of the two distributions into the orientations of Fig. 1. Then if $D^{(n)}(R)_{m'm}$ are the standard rotational representation coefficients, it follows that

$$\rho_{n_1m_1}(1;r_1)=\textstyle\sum_{m_1'}D^{(n_1)}(TS_1)_{m_1'm_1}\rho_{n_1m_1}{}'(1;r_1), \quad (9)$$

$$\rho_{n_2m_2}(2;r_2)=\textstyle\sum_{m_2'}D^{(n_2)}(TS_2)_{m_2'm_2}\rho_{n_2m_2}{}'(2;r_2). \quad (10)$$

Substituting Eqs. (9) and (10) into Eq. (6) gives V_{12} as a function of the orientations, TS_1 and TS_2, of the two charge distributions.

In quantum mechanics, the charge distributions only involve the first few spherical harmonics and, therefore, expansions of the form of Eq. (6) greatly simplify the work required in the evaluation of the coulombic integrals. As a matter of fact, most of the coulombic integrals are easy to evaluate once the B's are known. It is therefore worthwhile to evaluate the B's once and for all and thereby simplify a great many quantum-mechanical problems. The expansion, Eq. (1), can also be used to good advantage to determine the interaction between two discrete charge distributions. For example, the energy of interaction between two real dipoles as shown in Fig. 2 is given by the equation,

$$V_{12}=4e_1e_2\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\sum_{m=-(2n_<+1)}^{2n_<+1}B_{2n_1+1,\,2n_2+1}{}^{|m|}\times\left(\frac{l_1}{2},\frac{l_2}{2};R\right)\cdot P_{2n_1+1}{}^{|m|}(\cos\theta_1)P_{2n_2+1}{}^{|m|}(\cos\theta_2)\times\exp[im(\phi_2-\phi_1)]. \quad (11)$$

At distances, R, large compared with l_1 and l_2, the $B_{2n_1+1,\,2n_2+1}{}^{|m|}(l_1/2,l_2/2,R)$ vary as $R^{-3-2n_1-2n_2}$, so that the lead term, corresponding to $n_1=n_2=0$, is just the energy of interaction between two ideal dipoles.

THE FUNCTION $B_{n_1,n_2}{}^{|m|}(r_1,r_2;R)$

There are four sets of functional forms of the $B_{n_1n_2}{}^{|m|}$, corresponding to the four regions shown in Fig. 3:

$$\text{I. } R>r_1+r_2,\quad \text{II. } |r_1-r_2|\leqslant R\leqslant r_1+r_2,\quad \text{III. } r_2>R+r_1,\quad \text{IV. } r_1>R+r_2. \quad (12)$$

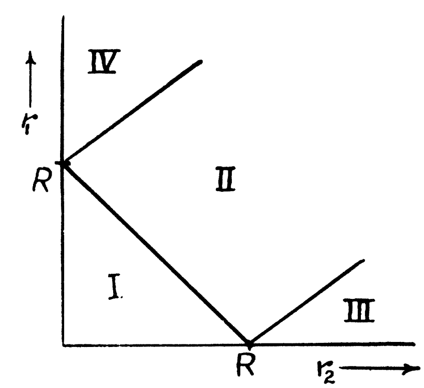

FIG. 3. The four regions of definition of the B's. I: $R>r_1+r_2$. II: $|r_1-r_2|\leqslant R\leqslant r_1+r_2$. III: $r_2>R+r_1$. IV: $r_1>R+r_2$.

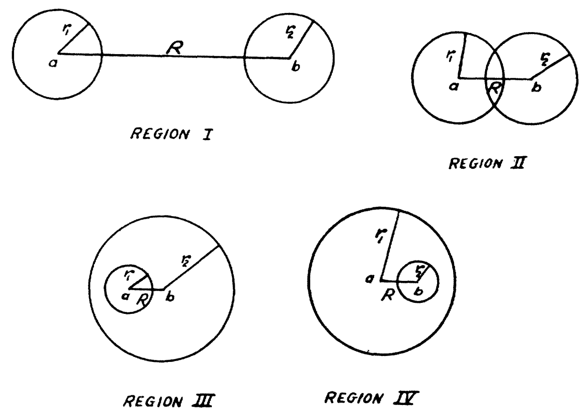

FIG. 4. Alternate description of the four regions. I: $R>r_1+r_2$. II: $|r_1-r_2|\leqslant R\leqslant r_1+r_2$. III: $r_2>R+r_1$. IV: $r_1>R+r_2$.

The geometrical significance of the four regions is shown in Fig. 4.

If the two charge distributions do not overlap, only region I need be considered. Here

Region I

$$B_{n_1,n_2}{}^{|m|}(r_1,r_2;R)=\frac{(-1)^{n_2+|m|}(n_1+n_2)!}{(n_1+|m|)!(n_2+|m|)!}r_1{}^{n_1}r_2{}^{n_2}R^{-n_1-n_2-1}. \quad (13)$$

For overlapping charge distributions it is necessary to consider the other three regions as well. In regions III and IV, the B's are still simple.[3]

Region III

$$B_{n_1,n_2}{}^{|m|}(r_1,r_2;R)=\frac{(-1)^{n_1+n_2}(n_2-|m|)!}{(n_1+|m|)!(n_2-n_1)!}\times r_1{}^{n_1}r_2{}^{-n_2-1}R^{n_2-n_1}\quad (n_2\geqslant n_1)$$
$$=0\quad (n_2<n_1). \quad (14)$$

Region IV

$$B_{n_1,n_2}{}^{|m|}(r_1,r_2;R)=\frac{(n_1-|m|)!}{(n_2+|m|)!(n_1-n_2)!}\times r_1{}^{-n_1-1}r_2{}^{n_2}R^{n_1-n_2}\quad (n_1\geqslant n_2)$$
$$=0\quad (n_1<n_2). \quad (15)$$

In Region II, the $B_{n_1,n_2}{}^m(r_1,r_2;R)$ are difficult to obtain. They have the functional form

Region II

$$B_{n_1,n_2}{}^{|m|}(r_1,r_2;R)=\frac{1}{D_{n_1,n_2}{}^{|m|}}\sum_{i,j=0}^{2(n_1+n_2+1)}A_{n_1,n_2}{}^{|m|}(i,j)\times r_1{}^{i-n_1-1}r_2{}^{j-n_2-1}R^{n_1+n_2-i-j+1}. \quad (16)$$

The coefficients $A_{n_1,n_2}{}^{|m|}$ and $D_{n_1,n_2}{}^{|m|}$ for n_1 and $n_2=0$, 1, 2, and 3 together with all of the appropriate values of m are given in Table I. The functions for which $n_1>n_2$ are not given, for they may be determined at once by permuting n_1 and n_2 according to the formula

$$B_{n_1,n_2}{}^{|m|}(r_1,r_2;R)=(-1)^{n_1+n_2}B_{n_2,n_1}{}^{|m|}(r_2,r_1;R). \quad (17)$$

For other values of n_1 and n_2 (not given in Table I), the coefficients may be evaluated by the methods discussed in the appendix.

Substituting Eqs. (13), (14), (15), and (16) into Eq. (6), the energy of interaction between two charge distributions may be written in the form:

$$V_{12}=V_{12}{}^{\mathrm{I}}+V_{12}{}^{\mathrm{II}}+V_{12}{}^{\mathrm{III}}+V_{12}{}^{\mathrm{IV}}, \quad (18)$$

where the $V_{12}{}^{\mathrm{I}}$, $V_{12}{}^{\mathrm{II}}$, $V_{12}{}^{\mathrm{III}}$, and $V_{12}{}^{\mathrm{IV}}$ are the contributions of the various regions:

$$V_{12}{}^{\mathrm{I}}=\sum_{n_1=0}^{\infty}\cdot\sum_{n_2=0}^{\infty}\sum_{m=-n_<}^{n_<}\frac{16\pi^2(-1)^{n_2+|m|}(n_1+n_2)!}{(2n_1+1)(2n_2+1)(n_1-|m|)!(n_2-|m|)!R^{1+n_1+n_2}}\cdot\int_0^R\rho_{n_2m}(2;r_2)r_2{}^{n_2+2}dr_2\int_0^{R-r_2}\rho_{n_1m}(1;r_1)r_1{}^{n_1+2}dr_1, \quad (19)$$

$$V_{12}{}^{\mathrm{II}}=\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\sum_{m=-n_<}^{n_<}\frac{16\pi^2(n_1+|m|)!(n_2+|m|)!}{(2n_1+1)(2n_2+1)(n_1-|m|)!(n_2-|m|)!D_{n_1n_2}{}^{|m|}}\sum_{i,j=0}^{2(n_1+n_2-1)}A_{n_1n_2}{}^{|m|}(i,j)R^{n_1+n_2+1-i-j}\left[\begin{array}{l}\displaystyle\int_0^R\rho_{n_2,m}(2;r_2)r_2{}^{j-n_2+1}dr_2\int_{R-r_2}^{R+r_2}\rho_{n_1,m}(1;r_1)r_1{}^{i-n_1+1}dr_1\\ \displaystyle+\int_R^\infty\rho_{n_2,m}(2;r_2)r_2{}^{j-n_2+1}dr_2\int_{r_2-R}^{r_2+R}\rho_{n_1,m}(1;r_1)r_1{}^{i-n_1+1}dr_1\end{array}\right], \quad (20)$$

[3] Carlson and Rushbrooke (reference 2) do not express the solution in this form, but Eqs. (14) and (15) follow from their results. An alternate derivation is given in the appendix.

$$V_{12}^{\mathrm{III}}=\sum_{n_2=0}^{\infty}\sum_{n_1=0}^{n_2}\sum_{m=-n_1}^{n_1}\frac{16\pi^2(-1)^{n_1+n_2}(n_2+|m|)!}{(2n_1+1)(2n_2+1)(n_1-|m|)!(n_2-n_1)!}R^{n_2-n_1}$$
$$\cdot\int_R^{\infty}\rho_{n_2,m}(2;r_2)r_2^{-n_2+1}dr_2\int_0^{r_2-R}\rho_{n_1,m}(1;r_1)r_1^{n_1+2}dr_1,\quad(21)$$

$$V_{12}^{\mathrm{IV}}=\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{n_1}\sum_{m=-n_2}^{n_2}\frac{16\pi^2(n_1+|m|)!R^{n_1-n_2}}{(2n_1+1)(2n_2+1)(n_2-|m|)!(n_1-n_2)!}$$
$$\cdot\int_0^{\infty}\rho_{n_2,m}(2;r_2)r_2^{n_2+2}dr_2\int_{R+r_2}^{\infty}\rho_{n_1,m}(1;r_1)r_1^{-n_1+1}dr_1.\quad(22)$$

If the first charge distribution is confined to a radius of l_1, and the second charge distribution is confined to a radius of l_2, then if R is larger than l_1+l_2 so that the charge distributions do not overlap, only V_{12}^{I} is different from zero and the energy of interaction has the form:

$$V_{12}=\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\sum_{m=-n_<}^{n_<}\frac{(-1)^{n_2+|m|}(n_1+n_2)!}{R^{1+n_1+n_2}}\times Q_{n_1,m}(1)Q_{n_2,m}(2),\quad(23)$$

where

$$Q_{n_1,m}(1)=\frac{4\pi}{(2n_1+1)(n_1-|m|)!}\times\int_0^{\infty}\rho_{n_1,m}(1;r_1)r_1^{n_1+2}dr_1,\quad(24)$$

$$Q_{n_2,m}(2)=\frac{4\pi}{(2n_2+1)(n_2-|m|)!}\times\int_0^{\infty}\rho_{n_2,m}(2;r_2)r_2^{n_2+2}dr_2.\quad(25)$$

In this way the energy of interaction is related to the moments of the charge distributions. Equation (18) is then, the generalization which applies to the overlapping charge distributions which are most common in quantum mechanics.

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APPENDIX. EVALUATION OF THE EXPANSION COEFFICIENTS

The reciprocal of the distance r_{12} between two points can be expressed by the well-known Neumann expansion.[4] Letting $(r_1,\ \theta_1,\ \varphi_1)$ and $(r_2',\ \theta_2',\ \varphi_2')$ be the spherical coordinates of the two points (with respect to origin a, as shown in Fig. 1) we have

$$\frac{1}{r_{12}}=\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\frac{(n-|m|)!}{(n+|m|)!}P_n^{|m|}(\cos\theta_1)P_n^{|m|}(\cos\theta_2')\times\exp[im(\phi_2'-\phi_1)]\frac{r_<^n}{r_>^{n+1}}.\quad(26)$$

Here $r_<$ is the lesser of r_2' and r_1 and $r_>$ is the greater of the two. The $P_n^m(\cos\theta)$ are the associated Legendre polynomials as defined by Eq. (2). The Neumann expansion converges provided that $r_{12}\neq 0$. Introducing the new origin, b, and new coordinates $(r_2,\ \theta_2,\ \varphi_2=\varphi_2')$ previously described, we may apply three identities given by Hobson:[5]

$$\frac{P_n^{|m|}(\cos\theta_2')}{(r_2')^{n+1}}=\sum_{k=|m|}^{\infty}\frac{(-1)^{|m|+k}(n+k)!}{(k+|m|)!(n-|m|)!}r_2^kR^{-n-k-1}\times P_k^{|m|}(\cos\theta_2)\quad(R>r_2),\quad(27)$$

$$\frac{P_n^{|m|}(\cos\theta_2')}{(r_2')^{n+1}}=\sum_{k=n}^{\infty}\frac{(-1)^{n+k}(k-|m|)!}{(k-n)!(n-|m|)!}r_2^{-k-1}R^{k-n}\times P_k^{|m|}(\cos\theta_2)\quad(R<r_2),\quad(28)$$

$$(r_2')^nP_n^{|m|}(\cos\theta_2')=\sum_{k=|m|}^{n}\frac{(n+|m|)!}{(k+|m|)!(n-k)!}\times r_2^kR^{n-k}P_k^{|m|}(\cos\theta_2).\quad(29)$$

Observing the inequalities, we see that these equations apply respectively in Region I ($r_2'>r_1$ and $R>r_2$), Region III ($r_2'>r_1$ and $R<r_2$), and Region IV ($r_2'<r_1$). On substituting into Eq. (26), we obtain the expansions given by Eqs. (1), (13), (14), and (15).

For Region II the coefficients may be given in terms of an integral. Equating r_{12}^{-1} from the Neumann

[4] See, for example, Eyring, Walter, and Kimball, *Quantum Chemistry* (John Wiley and Sons, Inc., New York, 1944), Appendix V.

[5] E. W. Hobson, *Theory of Spherical and Ellipsoidal Harmonics* (Cambridge University Press, London, 1931), Sec. 89.

TABLE I.* Expansion coefficients with indices $\leqslant 3$ for Region II. ($|r_1-r_2|\leqslant R\leqslant r_1+r_2$).

$$B_{n_1n_2}{}^m(r_1,r_2;R)=\sum_{i,j=0}^{2(n_1+n_2+1)}[A_{n_1n_2}{}^m(i,j)/D_{n_1n_2}{}^m]r_1{}^{i-n_1-1}r_2{}^{j-n_2-1}R^{n_1+n_2-i-j+1}.$$

The summation extends over all entries in the table.

	m	0	0	0	1	0	0	1	0
	n_1	0	0	1	1	0	1	1	0
	n_2	0	1	1	1	2	2	2	3
	$D_{n_1n_2}{}^m$	4	16	16	64	32	256	512	256
i	j	$A_{n_1n_2}{}^m(i,j)$							
0	0	−1	3	2	1	−5	−25	−5	35
	1	2	0	0	0	0	0	0	0
	2	−1	−6	−9	−9	5	60	20	−28
	3	0	0	8	16	0	0	0	0
	4	0	3	0	−9	5	−30	−30	−14
	6	0	0	−1	1	−5	−20	20	−28
	8	0	0	0	0	0	15	−5	35
1	0	2	−8	0	0	16	0	0	−128
	1	2	0	0	0	0	0	0	0
	3	0	−8	0	0	0	0	0	0
	5	0	0	0	0	16	0	0	0
	7	0	0	0	0	0	0	0	−128
2	0	−1	6	−9	−9	−15	180	60	140
	2	0	6	0	18	−10	−60	−60	84
	4	0	0	9	−9	−15	60	−60	84
	6	0	0	0	0	0	−180	60	140
3	0	0	0	8	16	0	−256	−128	0
	3	0	0	−16	16	0	0	0	0
	5	0	0	0	0	0	384	−128	0
4	0	0	−1	0	−9	5	90	90	−70
	2	0	0	9	−9	5	−60	60	−84
	4	0	0	0	0	0	−270	90	−70
6	0	0	0	−1	1	−1	20	−20	28
	2	0	0	0	0	0	60	−20	28
8	0	0	0	0	0	0	−9	3	−5

	m	0	1	2	0	1	0	1	2
	n_1	2	2	2	1	1	2	2	2
	n_2	2	2	2	3	3	3	3	3
	$D_{n_1n_2}{}^m$	256	1536	12288	256	1024	3072	12288	49152
i	j	$A_{n_1n_2}{}^m(i,j)$							
0	0	−19	−9	−3	21	7	189	49	7
	2	75	50	25	−42	−21	−630	−210	−42
	4	−150	−150	−150	14	14	735	315	105
	5	128	128	256	0	0	0	0	0
	6	−50	0	−150	0	14	−420	−140	−140
	8	25	−25	25	21	−21	315	−105	105
	10	−9	6	−3	−14	7	−294	126	−42
	12	0	0	0	0	0	105	−35	7
2	0	75	50	25	−210	−105	−1050	−350	−70
	2	−100	−100	−100	84	84	1470	630	210
	4	50	0	150	0	42	−420	−140	−140
	6	−100	100	−100	−84	84	−420	140	−140
	8	75	−50	25	210	−105	1470	−630	210
	10	0	0	0	0	0	−1050	350	−70
3	0	0	0	0	384	256	0	0	0
	7	0	0	0	−512	256	0	0	0
4	0	−150	−150	−150	−210	−210	3675	1575	525
	2	50	0	150	0	−126	−1260	−420	−420
	4	150	−150	150	126	−126	−630	210	−210
	6	−450	300	−150	420	−210	−2940	1260	−420
	8	0	0	0	0	0	7875	−2625	525
5	0	128	128	256	0	0	−4608	−2048	−1024
	5	768	−512	256	0	0	0	0	0
	7	0	0	0	0	0	−15360	5120	−1024
6	0	−50	0	−150	0	70	2100	700	700
	2	−100	100	−100	−84	84	1260	−420	420
	4	−450	300	−150	−140	70	2940	−1260	420
	6	0	0	0	0	0	10500	−3500	700
8	0	25	−25	25	21	−21	−525	175	−175
	2	75	−50	25	42	−21	−1470	630	−210
	4	0	0	0	0	0	−2625	875	−175
10	0	−9	6	−3	−6	3	294	−126	42
	2	0	0	0	0	0	630	−210	42
12	0	0	0	0	0	0	−75	25	−5

TABLE I.—(*Continued*).

	m	0	1	2	3
	n_1	3	3	3	3
	n_2	3	3	3	3
	$D_{n_1n_2}{}^m$	10240	49152	245760	2949120
i	j	$A_{n_1n_2}{}^m(i,j)$			
0	0	520	131	20	5
	2	−2450	−735	−147	−49
	4	4900	1715	490	245
	6	−7350	−2695	−1225	−1225
	7	5120	2048	1024	2048
	8	0	−735	0	−1225
	10	−1470	539	−245	245
	12	980	−343	98	−49
	14	−250	75	−15	5
2	0	−2450	−735	−147	−49
	2	5880	2058	588	294
	4	−4410	−1617	−735	−735
	6	0	588	0	980
	8	4410	−1617	735	−735
	10	−5880	2058	−588	294
	12	2450	−735	147	−49
4	0	4900	1715	490	245
	2	−4410	−1617	−735	−735
	4	0	294	0	490
	6	−2940	1078	−490	490
	8	14700	−5145	1470	−735
	10	−12250	3675	−735	245
6	0	−7350	−2695	−1225	−1225
	2	0	588	0	980
	4	−2940	1078	−490	490
	6	−19600	6860	−1960	980
	8	61250	−18375	3675	−1225
7	0	5120	2048	1024	2048
	7	−102400	30720	−6144	2048
8	0	0	−735	0	−1225
	2	4410	−1617	735	−735
	4	14700	−5145	1470	−735
	6	61250	−18375	3675	−1225
10	0	−1470	539	−245	245
	2	−5880	2058	−588	294
	4	−12250	3675	−735	245
12	0	980	−343	98	−49
	2	2450	−735	147	−49
14	0	−250	75	−15	5

* This table was checked in three ways: putting $(r_1, r_2; R) = (1, 1; 2)$, $(1, 2; 1)$, and $(2, 1; 1)$ we obtained values for the B's in agreement with those given by Eqs. (13), (14), and (15), respectively.

expansion, Eq. (26), to that from the bipolar expansion, Eq. (1); multiplying both sides of the equation by $P_{n_1}{}^{|m|}(\cos\theta_1)P_{n_2}{}^{|m|}(\cos\theta_2)\exp[im(\phi_2-\phi_1)]$ and integrating over the angles, it follows that

$$B_{n_1n_2}{}^{|m|}(r_1,r_2;R)=\left(\frac{2n_2+1}{2}\right)\frac{(n_2-|m|)!}{(n_2+|m|)!}\frac{(n_1-|m|)!}{(n_1+|m|)!}\cdot\int_{-1}^{1}\frac{r_<{}^{n_1}}{r_>{}^{n_1+1}}P_{n_1}{}^{|m|}(\cos\theta_2{}')P_{n_2}{}^{|m|}(\cos\theta_2)d(\cos\theta_2). \quad (30)$$

Here $r_<$ is the lesser of r_1 and $r_2{}'$ as before. In the integration over $\cos\theta_2$ we see that

$$r_2{}'<r_1 \quad \text{when} \quad -1<\cos\theta_2<-\cos\alpha, \quad (31)$$

$$r_2{}'>r_1 \quad \text{when} \quad -\cos\alpha<\cos\theta_2<1, \quad (32)$$

where

$$\cos\alpha=(R^2+r_2{}^2-r_1{}^2)/(2r_2R). \quad (33)$$

This situation is shown in Fig. 5. Thus in Region II,

Region II

$$B_{n_1n_2}{}^{|m|}(r_1,r_2;R)=\left(\frac{2n_2+1}{2}\right)\frac{(n_2-|m|)!}{(n_2+|m|)!}\frac{(n_1-|m|)!}{(n_1+|m|)!}$$
$$\cdot\left\{\int_{-1}^{-\cos\alpha}\frac{(r_2')^{n_1}}{r_1{}^{n_1+1}}P_{n_1}{}^{|m|}(\cos\theta_2')P_{n_2}{}^{|m|}(\cos\theta_2)d(\cos\theta_2)\right.$$
$$+\int_{-\cos\alpha}^{1}\frac{r_1{}^{n_1}}{(r_2')^{n_1+1}}P_{n_1}{}^{|m|}(\cos\theta'_2)$$
$$\left.\times P_{n_2}{}^{|m|}(\cos\theta_2)d(\cos\theta_2)\right\}. \quad (34)$$

Here

$$\cos\theta_2'=(r_2\cos\theta_2+R)/r_2', \quad (35)$$

$$r_2'=(R^2+r_2{}^2+2r_2R\cos\theta_2)^{\frac{1}{2}}. \quad (36)$$

We have not discovered a convenient method of evaluating the integrals of Eq. (34). The results given in Table I were determined by direct integration of the special cases. The Hobson expansions, Eqs. (27), (28), and (29) are no help for this purpose.

Convergence of the sum over n_2 follows from the fact that a constant$\times(r_<{}^n/r_>{}^{n+1})P_n{}^{|m|}(\cos\theta_2')$ is a bounded continuous function of $\cos\theta_2$ for $-1\leqslant\cos\theta_2\leqslant 1$ and therefore can be approximated by a series

$$\sum\nolimits_{n_2}B_{n_1n_2}{}^{|m|}P_{n_2}{}^{|m|}(\cos\theta_2).$$

Convergence of the sum over n_1 follows from convergence of the Neumann expansion.

The rule for permuting n_1 and n_2 in $B_{n_1n_2}{}^{|m|}(r_1,r_2;R)$, Eq. (17), can be derived in the following manner. Reverse the Z axis of the second charge distribution by defining $\theta_2^*=\pi-\theta_2$. Defining the new functions

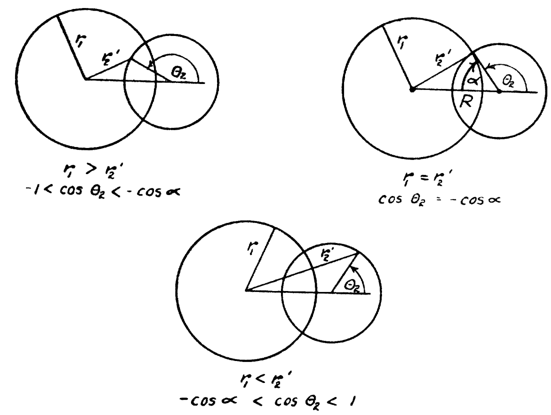

FIG. 5. Behavior of the ratio r_1/r_2' in the integration over $\cos\theta_2$.

$B_{n_1n_2}{}^{|m|*}(r_1,r_2;R)$ by the expansion,

$$\frac{1}{r_{12}}=\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\sum_{m=-n_<}^{n_<}B_{n_1n_2}{}^{|m|*}(r_1,r_2;R)P_{n_1}{}^{|m|}(\cos\theta_1)$$
$$\times P_{n_2}{}^{|m|}(\cos\theta_2^*)\exp[im(\phi_2-\phi_1)], \quad (37)$$

it follows from symmetry that in Region II

$$B_{n_1n_2}{}^{|m|*}(r_1,r_2;R)=B_{n_2n_1}{}^{|m|*}(r_2,r_1;R). \quad (38)$$

But $\cos\theta_2^*=-\cos\theta_2$ and

$$P_{n_2}{}^{|m|}(-\cos\theta_2)=(-1)^{n_2+m}P_{n_2}{}^{|m|}(\cos\theta_2),$$

so that comparing the expansions, Eqs. (1) and (37), and using Eq. (38),

$$B_{n_1n_2}{}^{|m|}(r_1,r_2;R)=(-1)^{n_2+|m|}B_{n_1n_2}{}^{|m|*}(r_1,r_2;R) \quad (39)$$
$$=(-1)^{n_2+|m|}B_{n_2n_1}{}^{|m|*}(r_2,r_1;R) \quad (40)$$
$$=(-1)^{n_2+n_1}B_{n_2n_1}{}^{|m|}(r_2,r_1;R). \quad (41)$$

This is proof of Eq. (17).