Useful alternative to the multipole expansion of $1/r$ potentials

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Few-body problems involving Coulomb or gravitational interactions between pairs of particles, whether in classical or quantum physics, are generally handled through a standard multipole expansion of the two-body potentials. We develop an alternative based on an old, but hitherto forgotten, expression for the inverse distance between two points that builds on azimuthal symmetry. This alternative should have wide applicability throughout physics and astronomy, both for computation and for the insights it provides through its emphasis on different symmetries and structures than are familiar from the standard treatment. We compare and contrast the two methods, develop addition theorems for Legendre functions of the second kind and a number of useful analytical expressions for these functions. Two-electron "direct" and "exchange" integrals in many-electron quantum systems are evaluated to illustrate the procedure, which is more compact than the standard one using Wigner coefficients and Slater integrals.

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I. INTRODUCTION

For pairwise Coulomb or gravitational potentials, one often expands the inverse distance between two points $\mathbf{x}$ and $\mathbf{x}'$ in the standard multipole form [1],

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|}=\frac{1}{\sqrt{rr'}}\sum_{\ell=0}^{\infty}\left(\frac{r_<}{r_>}\right)^{\ell+(1/2)}P_\ell(\cos\gamma), \tag{1.1}$$

where $r_<$ ($r_>$) is the smaller (larger) of the spherical distances r and r', and $P_\ell(\cos\gamma)$ is the Legendre polynomial [2] with argument

$$\cos\gamma\equiv\hat{\mathbf{x}}\cdot\hat{\mathbf{x}}'=\cos\theta\cos\theta'+\sin\theta\sin\theta'\cos(\phi-\phi'). \tag{1.2}$$

The set of six coordinates $\{\mathbf{x},\mathbf{x}'\}$ may be viewed either as defining two points relative to the origin or as the coordinates of a three-body system once the motion of the center of mass has been separated. In the "body frame," three out of the six coordinates are dynamical variables, the potential energy depending only on them. Of various choices for these variables, one is the set of three separation distances, another the triad ($r_<$, $r_>$, γ) as in Eq. (1.1). With respect to a space-fixed "laboratory frame," three more angles constitute the full set of six coordinates, the choice in Eq. (1.2) of (θ, θ', $\phi-\phi'$) being suited to the spherical polar coordinates of the individual vectors; thus, $\mathbf{x}=(r\sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta)$.

In this paper, we present an alternative expansion to Eq. (1.1) based on cylindrical (azimuthal) symmetry, which should be of wide interest in physics and astrophysics. This expansion arose in a recent investigation by two of us [3] of gravitational potentials in circular cylindrical coordinates $\mathbf{x}=(R,\phi,z)$,

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|}=\frac{1}{\pi\sqrt{RR'}}\sum_{m=-\infty}^{\infty}Q_{m-(1/2)}(\chi)e^{im(\phi-\phi')}, \tag{1.3}$$

where $Q_{m-(1/2)}$ is a Legendre function of the second kind of half-integer degree [4] and χ is defined as

$$\chi\equiv\frac{R^2+R'^2+(z-z')^2}{2RR'}=\frac{r^2+r'^2-2rr'\cos\theta\cos\theta'}{2rr'\sin\theta\sin\theta'}. \tag{1.4}$$

Although this expansion has been recorded in many places [5,6], its full significance has not been appreciated. We have traced its earliest occurrence to the work of E. Heine in the mid 19th century [5] and will, therefore, call it the "Heine identity." At its most general, it takes the form

$$\frac{1}{\sqrt{v-\cos\psi}}=\frac{\sqrt{2}}{\pi}\sum_{n=-\infty}^{\infty}Q_{n-(1/2)}(v)e^{in\psi}, \tag{1.5}$$

reducing to Eq. (1.3) when applied to the inverse distance between two points. We have found it to be a more efficient approach for problems with cylindrical geometry and regularly use it for compact numerical evaluation of gravitational-potential fields of axisymmetric and nonaxisymmetric mass distributions [3]. We now set Eq. (1.3) in a broader context, together with new associated addition theorems and a novel application in quantum physics, hoping to encourage wider use of this expansion throughout physics.

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II. THE ALTERNATIVE EXPANSIONS

The expansion in Eq. (1.1) disentangles the dynamics contained in the radial variables from symmetries, particularly under rotations and reflections pertaining to the angle γ. Whereas the three variables $\{r_<, r_>, \gamma\}$ at this stage are joint coordinates of $\mathbf{x}$ and $\mathbf{x}'$, a further disentangling in terms of the independent coordinates so as to handle permutational and rotational symmetry aspects of the problem, is often useful and achieved through the addition theorem for spherical harmonics [7],

$$P_\ell(\cos\gamma) = \frac{4\pi}{2\ell+1} \sum_{m=-\ell}^{\ell} Y_{\ell m}(\theta,\phi) Y_{\ell m}^*(\theta',\phi')$$

$$= \sum_{m=-\ell}^{\ell} \frac{\Gamma(\ell-m+1)}{\Gamma(\ell+m+1)} \times P_\ell^m(\cos\theta) P_\ell^m(\cos\theta') e^{im(\phi-\phi')}, \quad (2.1)$$

where $Y_{\ell m}$ are the standard spherical harmonics [7], $\Gamma(z)$ is the gamma function, and $P_\ell^m(z)$ is the integer-order, integer-degree, associated Legendre function of the first kind [2]. Using this to replace $P_\ell(\cos\gamma)$ in Eq. (1.1), we obtain the familiar Green's function multipole expansion in terms of all six spherical-polar-coordinate variables $\mathbf{x}$ and $\mathbf{x}'$,

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = \frac{1}{\sqrt{rr'}} \sum_{\ell=0}^{\infty} \left(\frac{r_<}{r_>}\right)^{\ell+1/2} \sum_{m=-\ell}^{\ell} \frac{\Gamma(\ell-m+1)}{\Gamma(\ell+m+1)} \times P_\ell^m(\cos\theta) P_\ell^m(\cos\theta') e^{im(\phi-\phi')}. \quad (2.2)$$

Apart from the first factor with dimension inverse distance formed from the geometric mean of the two lengths r and r', this expression involves only four combinations $(r_</r_>, \theta, \theta', \phi-\phi')$ of the six coordinates $\mathbf{x}$ and $\mathbf{x}'$. In spite of widespread familiarity with the multipole expansion, this reduction from six to four essential variables has not been appreciated fully. We were led to it by the parallel investigation below of the alternative expansion, and note that it is a natural consequence of the separation distance being independent of the orientation of that separation in the laboratory frame and thus independent of two angles serving to specify that orientation.

This multipole expansion in terms of spherical harmonics is very broadly utilized across the physical sciences. For example, with ℓ and m interpreted as the quantum numbers of orbital angular momentum and its azimuthal projection, respectively, a whole technology of Racah-Wigner or Clebsch-Gordan algebra is available [8] for handling all angular (that is, geometrical or symmetry) aspects of an N-body problem, the dynamics being confined to radial matrix elements of the coefficients $(r_</r_>)^{\ell+1/2}$ in Eq. (1.1). Although many other systems of coordinates have been studied for problems with an underlying symmetry that is different from the spherical, Eq. (1.1), in combination with the addition theorem for spherical harmonics, has gained such prominence as to have become the Green's function expansion of choice even for nonspherically symmetric situations.

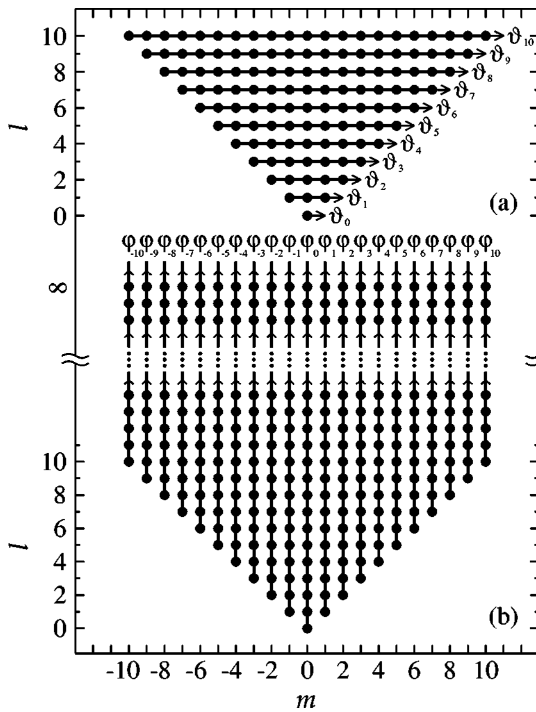

FIG. 1. Alternative double summations in (ℓ,m) space (a) first over m at fixed ℓ to form partial sums ϑ_ℓ as in Eq. (2.2), (b) first over ℓ at fixed m to form partial sums φ_m as in Eq. (2.3)

But, consider now the expansion in Eq. (1.3), which may be viewed either, in analogy with Eq. (1.1), as an expansion in Legendre functions, now of the second kind in the joint variable χ of the whole system, with coefficients $(RR')^{-1/2} e^{im(\phi-\phi')}$, or as a Fourier expansion in the variable $(\phi-\phi')$ with the Q's as coefficients. In this latter view, a further step allows us to develop a new addition theorem for these Legendre functions. Interchanging the ℓ and m summations (Fig. 1) in Eq. (2.2), we obtain

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = \frac{1}{\sqrt{rr'}} \sum_{m=-\infty}^{\infty} e^{im(\phi-\phi')} \sum_{\ell=|m|}^{\infty} \left(\frac{r_<}{r_>}\right)^{\ell+1/2} \times \frac{\Gamma(\ell-m+1)}{\Gamma(\ell+m+1)} P_\ell^m(\cos\theta) P_\ell^m(\cos\theta'). \quad (2.3)$$

Comparing with Eq. (1.3), we deduce

$$Q_{m-(1/2)}(\chi) = \pi\sqrt{\sin\theta\sin\theta'} \sum_{\ell=|m|}^{\infty} \left(\frac{r_<}{r_>}\right)^{\ell+(1/2)} \frac{\Gamma(\ell-m+1)}{\Gamma(\ell+m+1)} \times P_\ell^m(\cos\theta) P_\ell^m(\cos\theta'). \quad (2.4)$$

This is a new addition theorem for the Legendre function of the second kind. Note that $Q_{m-(1/2)} = Q_{-m-(1/2)}$ as per Eq. (8.2.2) in [2].

Similarities and contrasts between the pairs of equations, Eqs. (1.1) and (2.2) and Eqs. (1.3) and (2.3), are worth emphasizing. Of the four variables $(r_</r_>, \theta, \theta', \phi-\phi')$, the first pair of equations, Eqs. (1.1) and (2.2), expresses the inverse distance as a series in powers of the first variable with Legendre polynomials of the first kind in γ as coefficients, which is a composite of the other three variables and decomposable in terms of them through the addition theorem as in Eq. (2.1). The second pair of equations, Eqs. (1.3) and (2.3), on the other hand, expands in Eq. (1.3) the inverse distance in terms of the variable $\phi-\phi'$, with Legendre functions of the second kind in χ as expansion coefficients, which is a composite of the other three variables $(r_</r_>,\theta,\theta')$ and decomposable in terms of them through the addition theorem in Eq. (2.4). For this comparison, it is useful to recast Eq. (1.1) in the more suggestive form

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|}=\frac{1}{\sqrt{rr'}}\sum_{\ell=0}^{\infty}P_\ell(\cos\gamma)\times\exp\left[-\left(\ell+\frac{1}{2}\right)(\ln r_>-\ln r_<)\right]. \quad (2.5)$$

Whereas this expansion has half-integers in the exponents and integer-degree Legendre polynomials of the first kind as coefficients, Eq. (1.3) has integer m's as exponents and half-integer-degree Legendre functions of the second kind as coefficients.

Yet another alternative to Eq. (1.3) follows upon casting the square root in the expression for the distance in terms of r,r', and γ in the form of Eq. (1.5) through the definition

$$v\equiv\frac{1}{2}\left(\frac{r_<}{r_>}+\frac{r_>}{r_<}\right)=\frac{r^2+r'^2}{2rr'}. \quad (2.6)$$

This gives the expression

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|}=\frac{1}{\pi\sqrt{rr'}}\sum_{n=-\infty}^{\infty}Q_{n-(1/2)}(v)e^{in\gamma}, \quad (2.7)$$

now a Fourier expansion in γ instead of the angle $(\phi-\phi')$ of Eq. (1.3), with $Q_{n-(1/2)}(v)$ as the coefficients. In terms of hyperspherical coordinates, widely used in the atomic and nuclear study of three (or more) bodies [9], the variable v is $\csc 2\alpha$, α being a "hyperangle." In the Appendix, we present a number of alternative expressions for the functions $Q_{m-(1/2)}$, which we have found useful while working with the expansions in Eqs. (1.3) and (2.7).

III. TWO-ELECTRON INTEGRALS

One familiar application of expressions for the inverse distance is to the Coulomb interaction between two charges. We contrast usage of the alternative expansions in Eqs. (1.1) and (1.3) for calculating the electrostatic interaction as it appears in atomic, molecular, and condensed-matter physics. Thus, we consider the so-called "direct" part of this interaction between two electrons in the $3d^2$ configuration,

$$V_{ee}^D=\int d\mathbf{x}\int d\mathbf{x}'\,\psi_{3d}^*(\mathbf{x})\psi_{3d}^*(\mathbf{x}')\frac{1}{|\mathbf{x}-\mathbf{x}'|}\psi_{3d}(\mathbf{x})\psi_{3d}(\mathbf{x}'). \quad (3.1)$$

The standard treatment [10] uses Eqs. (1.1) and (2.3), carries out all the angular integrals through Racah-Wigner algebra, leaving behind radial "Slater integrals" $F^k(dd)$, $k=0,2,4$, and yielding (for illustrative purposes, all m values have been set equal to zero)

$$V_{ee}^D=F^0(dd)+(4/49)F^2(dd)+(36/441)F^4(dd), \quad (3.2)$$

where the coefficients are evaluated in terms of Wigner $3j$ symbols or are available in tables [10]. The Slater integrals,

$$F^k(dd)=\int\int r^2drr'^2dr'(r_<^k/r_>^{k+1})R_{3d}^2(r)R_{3d}^2(r'), \quad (3.3)$$

remain for numerical evaluation. In this example, upon evaluation with hydrogenic radial functions, we obtain $V=0.092\,172$ in atomic units.

The alternative calculation through Eq. (1.3) involves only the $m=0$ term and thereby the integral

$$V_{ee}^D=\frac{1}{\pi}\int\int\int\int R^{(1/2)}dRR'^{(1/2)}dR'dzdz'\times Q_{-(1/2)}(\chi)|\psi_{3d}(\mathbf{x})|^2|\psi_{3d}(\mathbf{x}')|^2. \quad (3.4)$$

The integrand is a function of z and R variables alone and our numerical evaluation of this integral reproduces the value cited above.

As a second example, we computed an exchange integral for the $3d4f$ configuration again setting, for simplicity, all m equal to zero,

$$V_{ee}^E=\int\int d\mathbf{x}d\mathbf{x}'\,\psi_{3d}^*(\mathbf{x})\psi_{4f}^*(\mathbf{x}')\frac{1}{|\mathbf{x}-\mathbf{x}'|}\psi_{3d}(\mathbf{x}')\psi_{4f}(\mathbf{x}). \quad (3.5)$$

The standard method through exchange Slater integrals G and Wigner coefficients gives [10]

$$V_{ee}^E=(9/35)G^1(df)+(16/315)G^3(df)+(500/7623)G^5(df) \quad (3.6)$$

and, again through hydrogenic radial functions, gives the value $V_{ee}^E=0.008\,286\,2$. We reproduce the same result upon directly computing Eq. (3.5) with Eq. (1.3), again involving a single four-dimensional integral as in Eq. (3.4) with $Q_{-1/2}$.

As the orbital angular momenta involved of the two electrons increase, the number of terms in expressions such as Eqs. (3.2) and (3.6) also grows, necessitating the computing of more Wigner coefficients and Slater integrals. By contrast, only a single term of the expansion in Eq. (1.3) and a single integral is necessary in our suggested alternative, the ϕ integrations setting $m=0$ for direct terms and m equal to the difference in the m values of the two orbitals for exchange terms. This same selection rule imposed by the ϕ integrations means that even in a calculation with several configurations and the imposition of antisymmetrization, such as in a multiconfiguration Hartree-Fock scheme, matrix elements of $|\mathbf{x}-\mathbf{x}'|^{-1}$ between each term in the bra and in the ket get a contribution from only one m value in the expansion in Eq. (1.3). This is a significant economy.

Although the evaluation of the four-dimensional integrals in Eq. (3.4) is computationally more demanding than the two-dimensional integrals of Eq. (3.3), the preparatory work of the Wigner-Racah algebra is avoided. A more efficient alternative to evaluating directly the four-dimensional integrals in expressions such as Eq. (3.4) is to use the fact that they can be viewed as electrostatic-interaction energies between charge densities given by the product of wave functions. The charge density $\rho(\mathbf{x}')$ is then used to find the potential at $\mathbf{x}$ and the resulting potential integrated with the appropriate charge density $\rho(\mathbf{x})$ to compute the integral [11]. This same approach applies to the decomposition according to Eq. (1.3) for each mth component of the potential. A two-dimensional Poisson equation in the primed variables in Eq. (3.4) is first solved and then Eqs. (3.4) and (3.5) are evaluated as two-dimensional integrals over the unprimed variables [12]. As already noted, direct integrals will involve only the $m=0$ component; exchange integrals involve a single m value equal to the difference in the azimuthal quantum numbers of the two orbitals.

IV. SUMMARY

The inverse distance between two points $\mathbf{x}'$ and $\mathbf{x}$ is intimately involved in Coulomb and gravitational problems. Its expansion in terms of Legendre polynomials P_ℓ of the angle between the vector pair or a further double-summation expansion involving the individual polar angles of the vectors are well known and widely used in physics and astronomy. We have discussed an alternative in terms of cylindrical coordinates, a single summation in terms of Legendre functions $Q_{m-1/2}$ of the second kind in a pair variable χ or double summations involving the individual coordinates. These expansions are better suited to problems that are decomposable in azimuthal symmetry as shown by applications in [3] and by an illustration here for very common electron-electron calculations throughout many-electron physics. Further variants are possible for other coordinates such as ring or toroidal, parabolic, bispherical, cyclidic and spheroidal [13], and we hope to return to them in future publications. Connections to the theory of Lie groups will also be of interest [14].

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APPENDIX: ALTERNATIVE EXPRESSIONS

We present in this appendix a number of alternative expressions for the functions $Q_{m-(1/2)}$, which are useful in calculations using expansions such as Eqs. (1.3) and (3.1). Setting $\theta=\theta'=\pi/2$ in Eq. (2.4) and using Eq. (8.756.1) of [15] gives

$$Q_{m-(1/2)}(v)=\pi\sum_{\ell=|m|}^{\infty}\left(\frac{r_<}{r_>}\right)^{\ell+(1/2)}\frac{\Gamma(\ell-m+1)}{\Gamma(\ell+m+1)}\times\frac{\pi 2^{2m}}{\left[\Gamma\left(1+\frac{\ell-m}{2}\right)\Gamma\left(\frac{1-\ell-m}{2}\right)\right]^2},\tag{A1}$$

which can be rewritten as

$$Q_{m-(1/2)}(v)=\pi e^{-(m+(1/2))\eta}\sum_{\ell=0}^{\infty}2^{1-2m-4\ell}\binom{2\ell}{\ell}\times\binom{2\ell+2m-1}{\ell+m}e^{-2\ell\eta},\tag{A2}$$

where we have defined $r_</r_>\equiv e^{-\eta}$, $v=\cosh\eta$. Although the ℓth term of these series is in a different form from what one obtains through the more familiar formula for Q as a hypergeometric function [16], namely,

$$Q_{m-(1/2)}(v=\cosh\eta)=\frac{\sqrt{\pi}\Gamma[m+(1/2)]}{\Gamma(m+1)}e^{-(m+(1/2))\eta}\times{}_2F_1\left(\frac{1}{2},m+\frac{1}{2};m+1;e^{-2\eta}\right),\tag{A3}$$

their equivalence follows from straightforward algebra. Also, another standard expansion for Q in powers of v as in Eq. (8.1.3) of [2],

$$Q_{\nu-(1/2)}(v)=\frac{\sqrt{\pi}\Gamma(\nu+(1/2))}{\Gamma(\nu+1)}(2v)^{-\nu-(1/2)}\times{}_2F_1\left(\frac{\nu}{2}+\frac{3}{4},\frac{\nu}{2}+\frac{1}{4};\nu+1;\frac{1}{v^2}\right),\tag{A4}$$

is equivalent. However, the results directly in powers of $r_</r_>$ in Eqs. (A1), (A2), and (A3) are more convenient in many applications. Among specific features worth noting in these alternative expansions are that only even powers of $(r_</r_>)$ occur in the sum in Eq. (A2) and that for any m, the sum in Eq. (A1) runs over all ℓ values compatible with it, $\ell\geqslant|m|$, as per their interpretation as angular momentum quantum numbers.

In the multipole expansion in Eq. (1.1), γ is an angle formed out of the set $(\theta,\theta',\phi-\phi')$ and, therefore, $\cos\gamma$ in the functions P_ℓ has a range of variation from -1 to 1. On the other hand, in the expansions in Eqs. (1.3) and (1.5), the arguments v and χ of the Legendre functions of the second kind range from 1 to ∞ and, therefore, can be written in terms of hyperbolic functions as $\cosh\eta$ and $\cosh\xi$, respectively. From Eq. (1.4) we have the link between them,

$$\cosh\eta = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cosh\xi. \tag{A5}$$

This disentanglement of v (or η) in terms of a triad is the counterpart of Eq. (1.2) and may be used with addition theorems given in the literature such as [5,6]

$$Q_{m-(1/2)}(\cosh\eta) = \sum_{n=-\infty}^{\infty} (-1)^n \frac{\Gamma\left(m-n-\frac{1}{2}\right)}{\Gamma\left(n+m-\frac{1}{2}\right)} \times Q^n_{m-(1/2)}(\cos\theta) P^n_{m-(1/2)}(\cos\theta') e^{n\xi}. \tag{A6}$$

An alternative to writing χ as $\cosh\xi$ is to set $\chi = \coth\zeta$ in Eq. (A5). In that case, it follows that

$$\exp\zeta \equiv \sqrt{\frac{\cosh\eta - \cos(\theta+\theta')}{\cosh\eta - \cos(\theta-\theta')}}. \tag{A7}$$

Other variants of the expansions in Eqs. (2.4) and (A6) follow from identities satisfied by the Legendre functions P and Q. In particular, there is an interesting pair of relations involving index interchange given in Eqs. (8.2.7) and (8.2.8) of [2],

$$Q^m_{n-(1/2)}(\cosh\eta) = (-1)^m \sqrt{\frac{\pi}{2\sinh\eta}} \times \Gamma\left(m-n+\frac{1}{2}\right) P^n_{m-(1/2)}(\coth\eta), \tag{A8}$$

$$Q^n_{m-(1/2)}(\coth\eta) = (-1)^m \sqrt{\frac{\pi\sinh\eta}{2}} \frac{\pi}{\Gamma\left(m-n+\frac{1}{2}\right)} \times P^m_{n-(1/2)}(\cosh\eta). \tag{A9}$$

[1] See, for instance, J. D. Jackson, *Classical Electrodynamics*, 2nd ed. (Wiley, New York, 1975), Sec. 4.1; H. Goldstein, *Classical Mechanics*, 2nd ed. (Addison-Wesley, Reading, 1980), Sec. 5.8; J. J. Sakurai, *Modern Quantum Mechanics* (Addison-Wesley, Reading, 1994), Sec. 6.4.
[2] See, for instance, *Handbook of Mathematical Functions*, Nat. Bur. Stand. Appl. Math. Ser. No. 55, edited by M. Abramowitz and I. A. Stegun (U.S. GPO, Washington, D.C., 1972), Chaps. 8 and 22.
[3] H. S. Cohl and J. E. Tohline, Astrophys. J. **527**, 86 (1999).
[4] See, for instance, A. Erdélyi, *Higher Transcendental Functions* (McGraw-Hill, New York, 1953) Vol. I, Chap. 3; *Handbook of Mathematical Functions* (Ref. [2]), Chap. 8.
[5] See, for instance, H. Bateman, *Partial Differential Equations of Mathematical Physics* (Cambridge University Press, New York, 1959), Sec. 10.2; E. Heine, *Handbuch der Kugelfunctionen* (Physica-Verlag, Wuerzburg, 1961), Vol. 2, Sec. 74.
[6] E. W. Hobson, *The Theory of Spherical and Ellipsoidal Harmonics* (Chelsea, New York, 1965), p. 443.
[7] J. D. Jackson, *Classical Electrodynamics* (Ref. [1]) Secs. 3.5 and 3.6; J. J. Sakurai, *Modern Quantum Mechanics* (Ref. [1]), Sec. 3.6.
[8] See, for instance, A. R. Edmonds, *The Quantum Theory of Angular Momentum* (Princeton University Press, Princeton, 1957); U. Fano and A. R. P. Rau, *Symmetries in Quantum Physics* (Academic, New York, 1996), Sec. 5.1; J. J. Sakurai, *Modern Quantum Mechanics* (Ref. [1]), Sec. 3.7.
[9] See, for instance, U. Fano and A. R. P. Rau, *Atomic Collisions and Spectra* (Academic, Orlando, 1986), Sec. 10.3.1; U. Fano and A. R. P. Rau, *Symmetries in Quantum Physics* (Ref. [8]), Sec. 10.2.2; C.D. Lin, Phys. Rep. **257**, 1 (1995).
[10] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, Cambridge, 1963), Sec. 8[6]. The entries in Table 1[6] for df, $k=5$ are in error and have been corrected in Eq. (3.6).
[11] See, for instance, L. D. Landau and E. M. Lifshitz, *Quantum Mechanics*, 3rd ed. (Pergamon, Oxford, 1977), p. 258; H. Friedrich, *Theoretical Atomic Physics*, 2nd ed. (Springer-Verlag, Berlin, 1998), Sec. 2.3.
[12] H. S. Cohl, X.-H.Sun, and Joel E. Tohline, in *Proceedings of the 8th SIAM Conference on Parallel Processing for Scientific Computing*, edited by M. Heath *et al.* (SIAM, Minneapolis, 1997); H.S. Cohl, Ph.D. dissertation, Louisiana State University, Baton Rouge, 1999.
[13] P. Moon and D. E. Spencer, *Field Theory Handbook: Including Coordinate Systems, Differential Equations and Their Solutions* (Springer-Verlag, Berlin, 1961), Chap. IV; H. S. Cohl, J. E. Tohline, A. R. P. Rau, and H. M. Srivastava, Astron. Nachr. **321**, 363 (2000).
[14] See, for instance, W. Miller, Jr., *Symmetry and Separation of Variables* (Addison-Wesley, London, 1977), Sec. 3.6; *Symmetry Groups and Their Applications* (Academic, New York, 1972); *Lie Theory and Special Functions* (Academic, New York, 1968).
[15] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products*, 5th ed. (Academic, New York, 1994).
[16] E. W. Hobson, *The Theory of Spherical and Ellipsoidal Harmonics* (Ref. [6]), p. 438.