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New complete orthonormal sets of hyperspherical harmonics and their one-range addition and expansion theorems

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Abstract In this study, the complete orthonormal sets of Φ^{α} - momentum space orbitals (where α=1,0,−1, −2,...) obtained from the Ψ^{α} -ETO in coordinate representation (I.I. Guseinov, J. Mol. Model., 9 (2003) 135) are reduced to the complete orthonormal sets of hyperspherical harmonics (HSH) by means of a Fock transformation of the radial momentum to an angular variable. It is shown that the group of transformations is the four-dimensional rotation group O (4) and, therefore, the HSH presented in this work are the complete orthonormal sets of functions. For these functions, the one-range addition and expansion theorems are obtained. The formulae for HSH and their addition and expansion theorems derived in this work can be used to evaluate the multicenter integrals that arise when exponential-type basis functions are used in atomic and molecular calculations.

Keywords Exponential-type orbitals · Hyperspherical harmonics · Multicenter integrals

Introduction

In [1], Fock reduced the Schrödinger equation of the hydrogen atom in momentum space to an integral equation in spherical harmonics in four variables by making a stereographic projection between momentum space and the four-dimensional unit sphere. This consideration is closely connected with the treatment of the hydrogen atom by the four-dimensional rotation group, which explains the degeneracy of the hydrogen levels with respect to the orbital quantum number. The connection of momentum-space quantum theory with HSH was made by Fock [1, 2]. He was able to show that the Fourier transforms of hydrogen-like orbitals can be expressed very simply in terms of HSH. However, it was realized that unless the continuum is included, the hydrogen-like orbitals and Fock's HSH are not complete. To achieve completeness, Shull and Löwdin [3] introduced a Coulomb Sturmian basis set, which is closely connected with the theory of HSH (see also [4, 5] and the bibliography quoted in these papers). They were able to show that this type of radial basis set is complete without the inclusion of the continuum. It is well known that the orthonormality relation obeyed by a Coulomb Sturmian basis set can be related, through Fock's transformation, to the orthonormality of HSH [6].

In [7, 8], Fock's method for HSH was extended to the multicenter one-electron problem by Shibuya and Wulfman (see also [9]). Unfortunately, convergence of the expansion derived by Shibuya and Wulfman is not guaranteed since the continuum states of the hydrogen spectrum are not included properly in the expansion. Recently, in [10] we introduced new complete orthonormal sets of Ψ^{α} -ETO in coordinate representation (where α=1,0,−1,−2,...), for which the problems with the continuum states do not occur. The complete orthonormal sets of Φ^{α} -momentum space orbitals (Φ^{α} -MSO) are defined as the Fourier transforms of Ψ^{α} -ETO in the momentum representation [11]. The aim of this work is to show that these Fourier transforms can be reduced to new complete orthonormal sets of four-dimensional HSH. It should be noted that the existence of HSH is equivalent to an additional symmetry of the screening Coulomb potentials beyond just invariance under spatial rotations.

Expressions for hyperspherical harmonics

The Fourier transforms of STO, Ψ^{α} -and $\overline{\Psi}^{\alpha}$ -ETO in momentum space are determined by [10, 11]:

$$U_{nlm}(\xi,\vec{k}) = (2\pi)^{-3/2}\int e^{-i\vec{k}\vec{r}}\chi_{nlm}(\xi,\vec{r})d^3\vec{r} = Q_{nl}(\xi,k)\widetilde{S}_{lm}(\theta,\varphi) \tag{1}$$

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$$\Phi^{\alpha}_{nlm}(\xi,\vec{k}) = (2\pi)^{-3/2}\int e^{-i\vec{k}\vec{r}}\Psi^{\alpha}_{nlm}(\xi,\vec{r})d^3\vec{r} = \Pi^{\alpha}_{nl}(\xi,k)\widetilde{S}_{lm}(\theta,\varphi) \quad (2)$$

$$\overline{\Phi}^{\alpha}_{nlm}(\xi,\vec{k}) = (2\pi)^{-3/2}\int e^{-i\vec{k}\vec{r}}\overline{\Psi}^{\alpha}_{nlm}(\xi,\vec{r})d^3\vec{r} = \overline{\Pi}^{\alpha}_{nl}(\xi,k)\widetilde{S}_{lm}(\theta,\varphi), \quad (3)$$

where $\overline{\Psi}^{\alpha}_{nlm}(\xi,\vec{r}) = (n/\xi r)^{\alpha}\Psi^{\alpha}_{nlm}(\xi,\vec{r})$ and the $\widetilde{S}_{lm}(\theta,\varphi) = (-i)^l S_{lm}(\theta,\varphi)$ is a modified spherical harmonic. We notice that the Ψ^{α} -ETO are orthonormal with $\overline{\Psi}^{\alpha}$ -ETO. The momentum space orbitals $Q_{nl}(\xi,k)$, $\Pi^{\alpha}_{nl}(\xi,k)$ and $\overline{\Pi}^{\alpha}_{nl}(\xi,k)$ occurring in Eqs. (1), (2), (3) are radial parts of the Fourier transforms:

$$Q_{nl}(\xi,k) = \frac{2^{n+l+1}l!(n-l)!}{\xi^{3/2}[\pi(2n)!]^{1/2}}x^{n+2}\left(1-x^2\right)^{l/2}C^{l+1}_{n-l}(x) \quad (4)$$

$$\Pi^{\alpha}_{nl}(\xi,k) = \sum_{\mu=l+1}^{n}\omega^{\alpha l}_{n\mu}Q_{\mu l}(\xi,k) \quad (5)$$

$$\overline{\Pi}^{\alpha}_{nl}(\xi,k) = (2n)^{\alpha}\sum_{\mu=l+1}^{n}\omega^{\alpha l}_{n\mu}\left[\frac{(2(\mu-\alpha))!}{(2\mu)!}\right]^{1/2}Q_{\mu-\alpha l}(\xi,k), \quad (6)$$

where $C^{l+1}_{n-l}(x)$ is a Gegenbauer polynomial and $x = \xi/(\xi^2+k^2)^{1/2}$. The quantities $\omega^{\alpha l}_{n\mu}$ in Eqs. (5) and (6) are the linear combination coefficients for the transformation of Ψ^{α} -ETO into STO determined by Eq. 7 of [10]. As can be seen from these formulae, the complete orthonormal sets of MSO are expressed in terms of Slater-type MSO by finite linear combinations.

Now we use the Fock's transformations in the following form:

$$\kappa_1 = \frac{k_x}{\sqrt{\xi^2+k^2}} = \sin\beta\cos\varphi\sin\theta \quad (7)$$

$$\kappa_2 = \frac{k_y}{\sqrt{\xi^2+k^2}} = \sin\beta\sin\varphi\sin\theta \quad (8)$$

$$\kappa_3 = \frac{k_z}{\sqrt{\xi^2+k^2}} = \sin\beta\cos\theta \quad (9)$$

$$\kappa_4 = \frac{\xi}{\sqrt{\xi^2+k^2}} = \cos\beta. \quad (10)$$

Here the angles β, θ, φ (where $0 \le \beta \le \frac{\pi}{2}$, $0 \le \theta \le \pi$, $0 \le \varphi \le 2\pi$) are spherical coordinates on the four-dimensional unit sphere; θ and φ have the meaning of the usual spherical coordinates in momentum space. The surface element of the four-dimensional sphere

$$d\Omega(\xi,\beta\theta\varphi) = \xi^3 d\Omega \quad (11)$$

is connected with the volume element in momentum space by the relation:

$$d^3\vec{k} = dk_x dk_y dk_z = d\Omega(\xi,\beta\theta\varphi), \quad (12)$$

where

$$d\Omega = d\Omega(1,\beta\theta\varphi) = \frac{\sin^2\beta}{\cos^4\beta}d\beta\sin\theta d\theta d\varphi. \quad (13)$$

Introducing the definitions in Eqs. (7), (8), (9), (10) into Eqs. (4), (5), (6) helps us to rewrite Eqs. (1), (2), (3) as

$$U_{nlm}\left(\xi,\vec{k}\right) = \frac{1}{\xi^{3/2}}V_{nlm}(\beta\theta\varphi) \quad (14)$$

$$\Phi^{\alpha}_{nlm}\left(\xi,\vec{k}\right) = \frac{1}{\xi^{3/2}}Z^{\alpha}_{nlm}(\beta\theta\varphi) \quad (15)$$

$$\overline{\Phi}^{\alpha}_{nlm}\left(\xi,\vec{k}\right) = \frac{1}{\xi^{3/2}}\overline{Z}^{\alpha}_{nlm}(\beta\theta\varphi). \quad (16)$$

Here, $V_{nlm}(\beta\theta\varphi) = U_{nlm}(1,\vec{k})$, $Z^{\alpha}_{nlm}(\beta\theta\varphi) = \Phi^{\alpha}_{nlm}(1,\vec{k})$ and $\overline{Z}^{\alpha}_{nlm}(\beta\theta\varphi) = \overline{\Phi}^{\alpha}_{nlm}(1,\vec{k})$ are the hyperspherical harmonics determined by

$$V_{nlm}(\beta\theta\varphi) = \Gamma_{nl}(\kappa_4)\widetilde{T}_{lm}(\kappa_1,\kappa_2,\kappa_3) \quad (17)$$

$$Z^{\alpha}_{nlm}(\beta\theta\varphi) = P^{\alpha}_{nl}(\kappa_4)\widetilde{T}_{lm}(\kappa_1,\kappa_2,\kappa_3) \quad (18)$$

$$\overline{Z}^{\alpha}_{nlm}(\beta\theta\varphi) = \overline{P}^{\alpha}_{nl}(\kappa_4)\widetilde{T}_{lm}(\kappa_1,\kappa_2,\kappa_3), \quad (19)$$

where

$$\Gamma_{nl}(\kappa_4) = \frac{2^{n+l+1}l!(n-l)!}{[\pi(2n)!]^{1/2}}\kappa_4^{n+2}C^{l+1}_{n-l}(\kappa_4) \quad (20)$$

$$P^{\alpha}_{nl}(\kappa_4) = \sum_{\mu=l+1}^{n} \omega^{\alpha l}_{n\mu} \Gamma_{\mu l}(\kappa_4) \tag{21}$$

$$\overline{P}^{\alpha}_{nl}(\kappa_4) = (2n)^{\alpha} \sum_{\mu=l+1}^{n} \omega^{\alpha l}_{n\mu} [\frac{(2(\mu-\alpha))!}{(2\mu)!}]^{1/2} \Gamma_{\mu-\alpha l}(\kappa_4) \tag{22}$$

$$\begin{aligned}\widetilde{T}_{lm}(\kappa_1,\kappa_2,\kappa_3) &= \sin^l \beta \left(\frac{4\pi}{2l+1}\right)^{1/2} \widetilde{S}_{lm}(\theta,\varphi) \\ &= (-i)^l \sum_{q=(|m|-m)/2}^{E\left(\frac{l-m}{2}\right)} \kappa_3^{l-m-2q} \sum_{\sigma=0}^{m+2q} A^{q\sigma}_{lm} \kappa_1^{m+2q-\sigma} \kappa_2^{\sigma}.\end{aligned} \tag{23}$$

Here, $E\left(\frac{l-m}{2}\right) = \frac{1}{2}\left[l - m - \frac{1}{2}\left(1-(-1)^{l-m}\right)\right]$ and the first three terms, Eqs. (20), (21), (22), correspond to the radial parts and the last one, Eq. (23), is the solid HSH. We notice that the new definitions for $V_{nlm}, Z^{\alpha}_{nlm}$ and $\overline{Z}^{\alpha}_{nlm}$ obtained from Eqs. (14), (15), (16) after setting ξ=1 correspond to the radius of the hyper-sphere on which the HSH are defined. The prove of Eq. (23) is presented in Appendix.

As can be seen from Eqs. (17), (18), (19), (20), (21), (22) the radial parts of hyperspherical harmonics $V_{nlm}(\beta\theta\varphi)$, $Z^{\alpha}_{nlm}(\beta\theta\varphi)$ and $\overline{Z}^{\alpha}_{nlm}(\beta\theta\varphi)$ obtained with the help of Fourier-Fock transforms of STO, Ψ^{α} - and $\overline{\Psi}^{\alpha}$ - ETO in coordinate representation are determined by the Gegenbauer polynomials. Their angular parts, the modified regular solid hyperspherical harmonics, Eq. (23), satisfy the Laplace equation.

Using Fock's transformations and the relations for the surface element of the four-dimensional sphere, Eqs. (11), (12), (13), one can show that the $V(\beta\theta\varphi)$ and $Z^{\alpha}_{nlm}(\beta\theta\varphi)$ are orthonormal with respect to the quantum numbers (l, m) and (n, l, m), respectively:

$$\int_0^{\pi/2}\int_0^{\pi}\int_0^{2\pi} V^*_{nlm}(\beta\theta\varphi) V_{\mu\nu\sigma}(\beta\theta\varphi) d\Omega = \delta_{l\nu}\delta_{m\sigma} \frac{(n+\mu)!}{\sqrt{(2n)!(2\mu)!}} \tag{24}$$

$$\int_0^{\pi/2}\int_0^{\pi}\int_0^{2\pi} Z^{\alpha *}_{nlm}(\beta\theta\varphi) \overline{Z}^{\alpha}_{\mu\nu\sigma}(\beta\theta\varphi) d\Omega = \delta_{n\mu}\delta_{l\nu}\delta_{m\sigma} \tag{25}$$

As we see from Eq. (15), the Fourier transformed Ψ^{α} -ETO are proportional to the four-dimensional spherical harmonics, i.e., to the Eigenfunctions for the four-dimensional quantal rotator problem. Thus, the Φ^{α} -MSO in Fock coordinates belong to spaces with different scales characterized by the parameter ξ. The parameter ξ is arbitrary in the region of positive real numbers (0<ξ<∞) and it is to be chosen as applied to a concrete problem. It should be noted that the sets of HSH, Eqs. (17), (18), (19), do not depend on the parameter ξ. The latter property acquires a special significance in the quantum theory of molecules, because addition and expansion theorems can be derived for hyperspherical harmonics. In particular, the Wigner–Biedenharn theorem [12] holds for the harmonics relevant to the rotation group O(4).

Addition and expansion theorems for hyperspherical harmonics

In order to derive the addition and expansion theorems for $V_{nlm}(\beta\theta\varphi)$ and $Z^{\alpha}_{nlm}(\beta\theta\varphi)$, we use Eqs. (1), (2), (14), (15) and the addition and expansion relations for $U_{nlm}\left(\xi,\vec{k}\right)$ and $\Phi^{\alpha}_{nlm}\left(\xi,\vec{k}\right)$ in momentum representation [11, 13]. Then, one gets the desired results:

Expansion theorems:

$$V^*_{nlm}(\beta\theta\varphi) V_{\mu\nu\sigma}(\beta\theta\varphi) = \frac{1}{2\pi} \sum_{N=1}^{n+\mu+1} \sum_{L=0}^{N-1} \sum_{M=-L}^{L} a^{\alpha NLM}_{nlm,\mu\nu\sigma} V^*_{NLM}(\beta\theta\varphi) \tag{26}$$

$$Z^{\alpha *}_{nlm}(\beta\theta\varphi) Z^{\alpha}_{\mu\nu\sigma}(\beta\theta\varphi) = \frac{1}{2\pi} \sum_{N=1}^{n+\mu+1} \sum_{L=0}^{N-1} \sum_{M=-L}^{L} d^{\alpha NLM}_{nlm,\mu\nu\sigma} Z^{\alpha *}_{NLM}(\beta\theta\varphi), \tag{27}$$

Addition theorems:

$$V_{nlm}(\beta_{k'}\theta_{k'}\varphi_{k'}) = 4\pi \sum_{\mu=1}^{\infty} \sum_{\nu=0}^{\mu-1} \sum_{\sigma=-\nu}^{\nu} \sum_{\mu'=\nu+1}^{\mu} \left(\sum_{N=1}^{n+\mu+1} \sum_{L=0}^{N-1} \sum_{M=-L}^{L} K^{\alpha NLM}_{nlm,\mu\nu\sigma}(\mu') V^*_{NLM}\left(\beta_p\theta_p\varphi_p\right) \right) V_{\mu'-\alpha\nu\sigma}(\beta_k\theta_k\varphi_k) \tag{28}$$

$$Z^{\alpha}_{nlm}(\beta_{k'}\theta_{k'}\varphi_{k'}) = 4\pi \sum_{\mu=1}^{\infty} \sum_{\nu=0}^{\mu-1} \sum_{\sigma=-\nu}^{\nu} \left(\sum_{N=1}^{n+\mu+1} \sum_{L=0}^{N-1} \sum_{M=-L}^{L} B^{\alpha NLM}_{nlm,\mu\nu\sigma} Z^{\alpha^*}_{NLM}(\beta_p\theta_p\varphi_p) \right) \overline{Z}^{\alpha}_{\mu\nu\sigma}(\beta_k\theta_k\varphi_k), \quad (29)$$

where α=1,0,−1,−2,... The Z^{α}_{nlm} and $\overline{Z}^{\alpha}_{nlm}$ are represented as finite linear combinations of $V_{\mu lm}$ by

$$Z^{\alpha}_{nlm}(\beta\theta\varphi) = \sum_{\mu=l+1}^{n} \omega^{\alpha l}_{n\mu} V_{\mu lm}(\beta\theta\varphi) \quad (30)$$

$$\overline{Z}^{\alpha}_{nlm}(\beta\theta\varphi) = (2n)^{\alpha} \sum_{\mu=l+1}^{n} \omega^{\alpha l}_{n\mu} [(2(\mu-\alpha))!/(2\mu)!]^{1/2} V_{\mu-\alpha lm}(\beta\theta\varphi) \quad (31)$$

and conversely,

$$V_{nlm}(\beta\theta\varphi) = \sum_{\mu=l+1}^{n} \overline{\omega}^{\alpha l}_{n\mu} Z^{\alpha}_{\mu lm}(\beta\theta\varphi). \quad (32)$$

Here, the four-dimensional angles ($\beta_k\, \theta_k\, \varphi_k$), ($\beta_p\, \theta_p\, \varphi_p$) and ($\beta_{k'}\, \theta_{k'}\, \varphi_{k'}$) can be determined from the components of momentum vectors $\overrightarrow{k}$, $\overrightarrow{p}$ and $\overrightarrow{k'} = \overrightarrow{k} - \overrightarrow{p}$, namely,

$$k_x = k\cos\varphi_k \sin\theta_k,\ k_y = k\sin\varphi_k \sin\theta_k,\ k_z = k\cos\theta_k \quad (33)$$

$$p_x = p\cos\varphi_p \sin\theta_p,\ p_y = p\sin\varphi_p \sin\theta_p,\ p_z = p\cos\theta_p \quad (34)$$

$$k'_x = k'\cos\varphi_{k'} \sin\theta_{k'},\ k'_y = k'\sin\varphi_{k'} \sin\theta_{k'},\ k'_z = k'\cos\theta_{k'}, \quad (35)$$

where $k = \sin\beta_k/\cos\beta_k$, $p = \sin\beta_p/\cos\beta_p$, $k' = \sin\beta_{k'}/\cos\beta_{k'}$ are the radial parts of momentum vectors $\overrightarrow{k}$, $\overrightarrow{p}$ and $\overrightarrow{k'}$, respectively.

The coefficients occurring in Eqs. (26), (27), (28), (29) are determined by the following relations:

$$a^{\alpha NLM}_{nlm,\mu\nu\sigma} = (-1)^{(l-\nu-L)/2}(2L+1)^{1/2} C^{L|M|}(lm,\nu\sigma) A^{M}_{m\sigma} \sum_{V=L+1}^{n+\mu+1} \Omega^{\alpha L}_{NV}(n+\mu+1) Q^{V-\alpha L}_{nl,\mu\nu} \quad (36)$$

$$d^{\alpha NLM}_{nlm,\mu\nu\sigma} = (-1)^{(l-\nu-L)/2}(2L+1)^{1/2} C^{L|M|}(lm,\nu\sigma) A^{M}_{m\sigma}(2N)^{\alpha} \times \sum_{n'=l+1}^{n} \sum_{\mu'=\nu+1}^{\mu} \sum_{V=L+1}^{N} \omega^{\alpha l}_{nn'} \omega^{\alpha\nu}_{\mu\mu'} \omega^{\alpha L}_{NV} \left[\frac{(2(V-\alpha))!}{(2V)!}\right]^{1/2} Q^{V-\alpha L}_{n'l,\mu'\nu} \quad (37)$$

$$K^{\alpha NLM}_{nlm,\mu\nu\sigma}(\mu') = (2\mu)^{\alpha}\left[\frac{(2(\mu'-\alpha))!}{(2\mu')!}\right]^{1/2} \omega^{\alpha\nu}_{\mu\mu'} \sum_{\mu''=l+1}^{n} \omega^{\alpha l}_{n\mu''} \sum_{N'=N}^{n+\mu+1} \omega^{\alpha L}_{N'N} B^{\alpha N'LM}_{\mu'' lm,\mu\nu\sigma} \quad (38)$$

$$B^{\alpha NLM}_{nlm,\mu\nu\sigma} = (-1)^{(l-\nu-L)/2}(2L+1)^{1/2} C^{L|M|}(lm,\nu\sigma) A^{M}_{m\sigma}(2N)^{\alpha} \times \sum_{n'=l+1}^{n} \sum_{\mu'=\nu+1}^{\mu} \sum_{V=L+1}^{N} \omega^{\alpha l}_{nn'} \omega^{\alpha\nu}_{\mu\mu'} \omega^{\alpha L}_{NV} \frac{(n'+\mu'+V-\alpha-1)!}{2^{n'+\mu'+1}[(2n')!(2\mu')!(2V)!]^{1/2}}. \quad (39)$$

See [10, 11, 13, 14] for the exact definition of parameters occurring in Eqs. (36), (37), (38), (39). It should be noted that the Eqs. (26), (27), (28), (29), (30), (31), (32), (33), (34), (35), (36), (37), (38), (39) for the multiplication and addition theorems were established with the help of complete orthonormal sets of Ψ^{α} -ETO and Φ^{α} -MSO (where α=1,0,−1,−2,...) introduced in our papers [10, 11], therefore, they are not available in the literature.

Summary

We have established the new complete orthonormal sets of hyperspherical harmonics $Z^{\alpha}_{nlm}(\beta\theta\varphi)$, where α=1,0,−1,−2,...

the group of transformations for which is the four-dimensional rotation group O(4). The addition and expansion theorems for these harmonics have been derived using properties of Ψ^{α} -ETO and Φ^{α} -MSO basis sets appearing in coordinate and momentum representations, respectively. The Z^{α} -HSH are expressed in terms of V-HSH obtained from STO in momentum space by the linear combinations. The complete orthonormal sets of functions and their one-range addition and expansion theorems presented in this work, and in [10, 11, 13] for the Ψ^{α} -ETO, Φ^{α} -MSO and Z^{α} -HSH in coordinate, momentum and four-dimensional spaces, respectively, can be useful in the study of different problems appearing in quantum mechanics.

Appendix

We have seen above that the HSH are expressed through the modified regular solid HSH of the unit sphere determined by Eq. (23). In order to derive Eq. (23) we use the following relation for the complex regular solid spherical harmonics (see Equation (5.1.16) in [15]):

$$\begin{aligned} T_{lm}(x,y,z) &= \left(\frac{4\pi}{2l+1}\right)^{1/2} r^l Y_{lm}(\theta,\varphi) \\ &= (-1)^{(|m|+m)/2}[(l+m)!(l+m)!]^{1/2} \\ &\times \sum_{pqs} \frac{1}{p!q!s!}\left(-\frac{x+iy}{2}\right)^p \left(\frac{x-iy}{2}\right)^q z^s, \end{aligned} \tag{40}$$

where $p+q+s=l$ and $p-q=m$. Then taking into account the expansion relation

$$(x+y)^n(x-y)^{n'} = \sum_{m=0}^{n+n'} F_m(n,n')x^{n+n'-m}y^m \tag{41}$$

for the binomial product in Eq. (40) and the properties of complex and real spherical harmonics it is easy to prove Eq. (23) for solid HSH.

The coefficients $A_{lm}^{q\sigma}$ occurring in Eq. (23) are determined by the relations:
for complex spherical harmonics

$$\begin{aligned} A_{lm}^{q\sigma} &= \frac{1}{2^{m+2q}}[(-1)^{\sigma/2} + i(-1)^{(\sigma-1)/2}](-1)^{q+(|m|-m)/2} \\ &\left(F_l(l+|m|)/F_{l-|m|}(l)\right)^{1/2} \times F_q(l-m-q) \\ &F_{m+q}(l)F_\sigma(m+q,q), \end{aligned} \tag{42}$$

for real spherical harmonics

$$\begin{aligned} A_{lm}^{q\sigma} &= \frac{1}{2^{m+2q}}(-1)^{q+\left(|m|-m+\sigma+\Delta_{m,-|m|}\right)/2}((2-\delta_{m0}) \\ &F_l(l+|m|)/F_{l-|m|}(l))^{1/2} \times F_q(l-m-q) \\ &F_{m+q}(l)F_\sigma(m+q,q). \end{aligned} \tag{43}$$

Here

$$\Delta_{m,-|m|} = \begin{cases} 0 & for \quad m \geq 0 \\ 1 & for \quad m < 0 \end{cases} \tag{44}$$

$$F_k(n) = \begin{cases} n!/[k!(n-k)!] & for \quad 0 \leq k \leq n \\ 0 & for \quad k < 0, k > n \end{cases} \tag{45}$$

$$F_k(n,n') = \sum_\sigma (-1)^\sigma F_{k-\sigma}(n)F_\sigma(n'), \tag{46}$$

where $\frac{1}{2}[(k-n)+|k-n|] \leq \sigma \leq \min(k,n')$ and $F_k(n) \equiv F_k(n,0)$. The symmetry properties of $F_k(n, n')$ are given in [14].

We notice that the definition of phases in Eq. (40) for the complex spherical harmonics $\left(Y_{lm}^* = Y_{l-m}\right)$ differs from the Condon–Shortley phases [16] by the sign factor $(-1)^m$.

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