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Expansion of a function about a displaced center

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A simpler, more general version of a formula given by Sharma for the expansion of functions of the form, $F(\vec{r}) = f(r)Y_l^m(\theta,\phi)$, in terms of spherical harmonics and radial functions at a new origin, is derived from an earlier treatment of the expansion problem based on Fourier transforms.

Recently Sharma[1] re-examined the problem of expressing a function of the form $F(\vec{r})=f(r)Y_L^M(\theta,\phi)$ in terms of spherical harmonics and radial functions at a new origin. He obtained a formula for the new radial function as a quadrature involving the old radial function. We wish to give here a simpler and more general formula, based on our earlier treatment of the expansion problem using Fourier transforms.[2]

The formula we wish to establish is, in the notation of Ref. 2,

$$F(\vec{r}-\vec{R})=\sum_{\substack{l=0\\(l+L+\lambda\text{ even})}}^{\infty}\;\sum_{\lambda=|l-L|}^{l+L} v_{l\lambda L}(r,R)\times\sum_{M=-l}^{l} C_{\lambda LMlm}Y_\lambda^{M-m}(\theta_R,\phi_R)Y_l^m(\theta,\phi)\,, \quad (1)$$

$$C_{\lambda LMlm}=\int d\Omega\, Y_\lambda^{M-m*}(\theta,\phi)Y_l^{m*}(\theta,\phi)Y_L^M(\theta,\phi)\,, \quad (2)$$

$$v_{l\lambda L}(r,R)=2\pi(-1)^l R^{-1}\times\sum_{s=0}^{(L+l+\lambda)/2}\;\sum_{t=0}^{(L+l+\lambda)/2-s} D_{l\lambda Lst}\left(\frac{r}{R}\right)^{2t-l-1}\times\int_{|r-R|}^{r+R} dr'\left(\frac{r'}{R}\right)^{2s-L+1} f(r')\,, \quad (3)$$

$$D_{l\lambda Lst}=[(2s)!!(2s-2L-1)!!(2t)!!(2t-2l-1)!!\times(L+l+\lambda-2s-2t)!!\times(L+l-\lambda-2s-2t-1)!!]^{-1}\,. \quad (4)$$

This formula is more general than Sharma's [Eqs. (1), (16a), and (17a)–(17d) of Ref. 1] in that the vector from the old origin to the new one, $\vec{R}$, need not lie along the z axis. At the same time it is simpler, in that the use of the well-known quantity $C_{\lambda LMlm}$ of Eq. (2)—formulas for which appear in many standard references[3,4]—replaces three summations in Sharma's Eq. (17b).

The derivation of Eqs. (1)–(4) is given, save for one final step, in Eqs. (20), (21), (17), and (18) of our earlier paper,[2] which gives Eqs. (1) and (2), but instead of Eqs. (3) and (4), the pair of equations

$$v_{l\lambda L}(r,R)=\pi^{-1}i^{\lambda-l}\int_{-\infty}^{\infty} dk\,k^2 j_\lambda(kR)j_l(kr)\overline{\psi}(k)\,, \quad (5)$$

$$\overline{\psi}(k)=4\pi i^L\int_0^\infty dr'\,r'^2 f(r')j_L(kr')\,. \quad (6)$$

Here, $j_l(x)$ is the usual spherical Bessel function. Substitution of Eq. (6) into Eq. (5) and interchange of the two integrations,

$$v_{l\lambda L}(r,R)=4(-1)^{(l-\lambda-L)/2}\int_0^\infty dr'\,r'^2 f(r')\times\int_{-\infty}^{\infty} dk\,k^2 j_\lambda(kR)j_l(kr)j_L(kr')\,, \quad (7)$$

leads to an integral over a triple product of spherical Bessel functions that is closely related to one that occurs in the derivation of the bipolar expansion formula[5] for $r^N Y_L^M$, and that can be similarly evaluated by contour integration. The result,

$$\int_{-\infty}^{\infty} dk\,k^2 j_\lambda(kR)j_l(kr)j_L(kr')=\tfrac{1}{2}(-1)^{(l+\lambda+L)/2}\pi R^{-3}\sum_{s=0}^{(L+l+\lambda)/2}\;\sum_{t=0}^{(L+l+\lambda)/2-s} D_{l\lambda Lst}\left(\frac{r}{R}\right)^{2t-l-1}\left(\frac{r'}{R}\right)^{2s-L-1}\,,\quad |r-r|<r'<r+R\,, \quad (8)$$

$$=0\,,\quad r'<|r-R| \text{ or } r'>r+R\,, \quad (9)$$

when substituted into Eq. (7), yields Eqs. (3) and (4).

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[2]H. J. Silverstone, J. Chem. Phys. 47, 537 (1967).
[3]J. A. Gaunt, Philos. Trans. R. Soc. Lond. A 228, 151 (1929).
[4]E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University, London, 1935), Chap. 6, Sec. 8.
[5]K. G. Kay, H. D. Todd, and H. J. Silverstone, J. Chem. Phys. 51, 2363 (1969), especially Eq. (6).