Addition Theorems & Green’s Functions

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Abstract

The spherical harmonics $Y_l^m(\hat{\boldsymbol{u}})$, where $\hat{\boldsymbol{u}}$ is a 3D unit vector, are familiar to chemists and physicists, arising as joint eigenfunctions of the square of the orbital angular momentum operator $\mathbb{L}^2$ and the generator of rotations about the azimuthal axis $\mathbb{L}_z$:

$$\mathbb{L}^2\, Y_l^m(\hat{\boldsymbol{u}}) = l\,(l+1)\, Y_l^m(\hat{\boldsymbol{u}}),\ \ l = 0,\ 1,\ 2,\ \ldots$$

$$\mathbb{L}_z\, Y_l^m(\hat{\boldsymbol{u}}) = m\, Y_l^m(\hat{\boldsymbol{u}}),\ \ m = -l,\ -1+1,\ \ldots,\ l-1,\ l.$$

The $Y_l^m(\hat{\boldsymbol{u}})$ provide a representation of the symmetry group of rotations around a point and satisfy a simple addition theorem

$$\sum_m Y_l^m(\hat{\boldsymbol{u}})^*\, Y_l^m(\hat{\boldsymbol{v}}) = \frac{2\,l+1}{4\,\pi}\, P_l(\hat{\boldsymbol{u}}\cdot\hat{\boldsymbol{v}}),$$

where $P_l(x)$ is a Legendre polynomial.

The generalised Green's function $G_n(x)$ satisfies

$$\left(\mathbb{L}^2 - n\,(n+1)\right) G_n(\hat{\boldsymbol{u}}\cdot\hat{\boldsymbol{v}}) = \delta(1 - \hat{\boldsymbol{u}}\cdot\hat{\boldsymbol{v}}) - \frac{2\,n+1}{4\,\pi}\, P_n(\hat{\boldsymbol{u}}\cdot\hat{\boldsymbol{v}}),$$

and can be computed in closed-form by term-by-term inversion,

$$G_n(x) = \frac{1}{2\,\pi}\left(\sum_{l=0}^{n-1} \frac{(2\,l+1)\,P_l(x)}{(l-n)\,(l+n+1)} - \frac{1}{2}\log\left(\frac{1-x}{2}\right) P_n(x)\right).$$

Here we will examine rotations and spherical harmonics in both 4D and 6D, present a simple derivation of the associated addition theorems and related generalised Green’s functions, with application to exact solution of the Fock (1954, 1958) expansion for Helium.

References

1. Fock, VA 1954 ‘On the Schrödinger Equation of the Helium Atom’ Izv Akad Nauk SSSR Ser Fiz, 18:161–174
2. Fock, VA 1958 ‘On the Schrödinger Equation of the Helium Atom’ Kgl Norske Vidensk Selsk Skr 31(22):138-144 and 31(23):145-152