SPHERICAL HARMONICS VIA KRAMER’S METHOD

Note: \( Y(\theta,\phi) \) is independent of \( E \) and \( V \).

Thus we can solve for the case \( E = V(r) \) with \( r = \text{constant} \), take just

\[
\nabla^2 \psi = 0 \quad \text{totally determined Laplace equation due to the symmetry of the problem}
\]

The solutions of the angular part in spherically symmetric problems are well known in classical physics (and have nothing to do with quantum mechanics). Thus, e.g., we can expand a general function in spherical harmonics just as with the Fourier series.

The following method of constructing the \( Y(\theta,\phi) \) functions is due to Kramers. Represent solutions of Laplace equation by a power series,

\[
\psi_\ell = \sum_{p+q+r=\ell} a_{pqr} x^p y^q z^r
\]

where we require \( p+q+r = \ell \) in order that \( \psi_\ell \) have the form

\[
\psi_\ell = R(r)Y(\theta,\phi).
\]

In fact, \( \psi_\ell = \text{const.} \cdot r^\ell Y(\theta,\phi) \) since \( \begin{cases} x = rsin\theta cos\phi \\ y = rsin\theta sin\phi \\ z = rcos\phi \end{cases} \)

we choose the coefficients \( a_{pqr} \) to satisfy \( \nabla^2 \psi = 0 \).

Consider solutions for each \( \ell \) in succession:

\[ \ell = 0 \]

\[
\psi_0 = \text{const.} \quad \text{only solution}
\]

\[ \ell = 1 \]

\[
\psi_1 = ax + by + cz \quad \text{satisfies} \quad \nabla^2 \psi_1 = 0 \quad \text{for any arbitrary choices of} \ a, b, c, \ \text{so there are 3 independent solutions}
\]

\[ \ell = 2 \]

\[
\psi_2 = ax^2 + by^2 + cz^2 + dxy + eyz + fzx
\]

Now \( \nabla^2 \psi_2 = 0 \) requires \( 2(a+b+c) = 0 \). Thus there is one condition on the 6 parameters, so there are only 5 independent solutions.

\[ \ell = 3 \]

\[
\psi_3 = ax^3 + by^3 + cz^3 + dx^2y + ex^2z + fxy^2 + fyz^2 + hzx^2 + iyz^2 + jxyz
\]

\( \nabla^2 \psi_3 = 0 \) requires \( 6ax + 6by + 6cz + 2dy + 2ez + 2fx + 2gz + 2hx + 2iy = 0 \)

Since \( x, y, z \) are independent variables, this requires

\[
\begin{align*}
6a + 2f + 2h &= 0 \\
6b + 2d + 2i &= 0 \\
6c + 2e + 2g &= 0
\end{align*}
\]

Now there are 3 conditions on 10 parameters, so there are only 7 independent solutions.
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General Case: For a given \( \ell \), the number of terms \( x^p y^q z^r \) in \( \psi_\ell \) is \( \frac{1}{2}(\ell+1)(\ell+2) \). But \( \nabla^2 \psi_\ell \) is a polynomial of degree \( \ell-2 \), so the requirement that \( \nabla^2 \psi_\ell = 0 \) imposes \( \frac{1}{2}(\ell-1)\ell \) conditions. Thus there remain

\[
\frac{1}{2}(\ell+1)(\ell+2) - \frac{1}{2}(\ell-1)\ell = 2\ell + 1
\]

linearly independent polynomials of degree \( \ell \).

NOTE: How many linearly independent terms of the form \( x^p y^q z^r \) with \( n_x + n_y + n_z = N \)? In \( n_x, n_y, n_z \) space this condition defines a plane:

There are \( N+1 \) planes of the form \( n_z = k \) which will intersect the plane \( N = n_x + n_y + n_z \). The number of points (i.e. allowed solutions) contained in these intersections are:

For \( n_z = N \): 1

\( n_z = k \): \( N - k + 1 \)

\( n_z = 0 \): \( N + 1 \)

Thus the total degeneracy is

\[
\sum_{k=0}^{N} (N+1-k) = N(N+1) + 1 \cdot (N+1) + \sum_{k=0}^{N} (-k)
\]

\[
= (N+1)^2 - \sum_{k=1}^{N} k
\]
We are free to choose the form of the linearly independent polynomials, we will take them to be orthogonal. Thus we use:

- \( l = 0 \): 1
- \( l = 1 \): \( x, y, z \)
- \( l = 2 \): \( xy, yz, zx, x^2 - y^2, 2z^2 - x^2 - y^2 \)
- \( l = 3 \): \( x(x^2 - 3z^2), x(x^2 - 3y^2), y(y^2 - 3x^2), y(y^2 - 3z^2), \)
  \( z(z^2 - 3x^2), z(z^2 - 3y^2), xyz \)
  etc.

In each case, the solution has the form \( \psi_\ell = r^\ell Y_\ell(\theta, \phi) \). Hence we have

\[
\nabla^2 \psi_\ell = \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi_\ell}{\partial r} \right) - \frac{\ell(\ell + 1) - C}{r^2} \right] \psi_\ell
\]

\[
= [\ell(\ell + 1) - C] \frac{1}{r^2} \psi_\ell
\]

\( \Rightarrow C = \ell(\ell + 1) \)

\( \psi_\ell(\theta, \phi) = \psi_\ell/r^\ell \) is a spherical harmonic of order \( \ell \).