

SPHERICAL HARMONICS - EXAMPLES

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.3.

In the solution of the 3-d Schrödinger equation with a radial potential, we found that the angular part could be written in terms of spherical harmonics

$$(0.1) \quad Y_l^m(\theta, \phi) = \varepsilon \left[\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!} \right]^{1/2} e^{im\phi} P_l^m(\cos \theta)$$

with $\varepsilon = (-1)^m$ for $m > 0$ and $\varepsilon = 1$ for $m < 0$ and the P_l^m being the associated Legendre function:

$$(0.2) \quad P_l^m(x) = (1-x^2)^{m/2} \sum_{k=0}^{[(l-m)/2]} \frac{(2l-2k)!}{2^l(l-k)!k!(l-2k-m)!} (-1)^k x^{l-m-2k}$$

As an example, we can calculate a couple of the spherical harmonics from these formulas.

Y_0^0 can be calculated easily from inspection of the formulas and comes out to

$$(0.3) \quad Y_0^0 = \left(\frac{1}{4\pi} \right)^{1/2}$$

To get Y_2^1 , we start with 0.1:

$$(0.4) \quad Y_2^1 = -\sqrt{\frac{5}{24\pi}} e^{i\phi} P_2^1(\cos \theta)$$

Then from 0.2

$$(0.5) \quad P_2^1(x) = (1-x^2)^{1/2} \sum_{k=0}^{[1/2]} \frac{(4-2k)!}{2^2(2-k)!k!(2-2k-1)!} (-1)^k x^{1-2k}$$

$$(0.6) \quad = (1-x^2)^{1/2} (3x)$$

$$(0.7) \quad P_2^1(\cos \theta) = 3 \sin \theta \cos \theta$$

So finally we get

$$(0.8) \quad Y_2^1(\theta, \phi) = -\sqrt{\frac{15}{8\pi}} e^{i\phi} \sin \theta \cos \theta$$

The normalization can be checked by direct integration

$$(0.9) \quad \int_0^{2\pi} \int_0^\pi |Y_0^0|^2 \sin \theta d\theta d\phi = \int_0^{2\pi} \int_0^\pi \frac{1}{4\pi} \sin \theta d\theta d\phi$$

$$(0.10) \quad = 1$$

$$(0.11) \quad \int_0^{2\pi} \int_0^\pi |Y_2^1|^2 \sin \theta d\theta d\phi = \frac{15}{8\pi} \int_0^{2\pi} \int_0^\pi \sin^3 \theta \cos^2 \theta d\theta d\phi$$

$$(0.12) \quad = \frac{1}{2\pi} \int_0^{2\pi} d\phi$$

$$(0.13) \quad = 1$$

The orthogonality can be checked in a similar way, by direct integration

$$(0.14)$$

$$\int_0^{2\pi} \int_0^\pi (Y_0^0)^* Y_2^1 \sin \theta d\theta d\phi = \sqrt{\frac{15}{32\pi^2}} \int_0^{2\pi} \int_0^\pi e^{i\phi} \sin^2 \theta \cos \theta d\theta d\phi$$

$$(0.15) \quad = 0$$

where the zero results from the first integral over θ .

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