SPHERICAL HARMONICS

Def. A function $f : \mathbb{R}^n \to \mathbb{R}$ is homogeneous of degree k if and only if

$$f(tx) = t^k f(x), \quad \forall x \in \mathbb{R}^n, \ t > 0.$$

Def. $P_k(n+1)$ = set of homogeneous polynomials of degree k in $n+1$ variables.

$\mathcal{H}_k(n+1)$ = set of harmonic polynomials with k-homogeneity
$= \{ P \in P_k(n+1) : \Delta P = 0 \}$
(= solid harmonics)

Def. $\mathcal{H}_k(S^n)$ = the space of spherical harmonics given by restricting harmonic polynomials to S^n.

Lemma. There is a linear isomorphism

$$\mathcal{H}_k(n+1) \xrightarrow{\simeq} \mathcal{H}_k(S^n).$$

Proof. If $P \in \mathcal{H}_k(n+1)$ then $P(x) = |x|^k P\left(\frac{x}{|x|}\right)$, $\frac{x}{|x|} \in S^n$, $x \neq 0$.

So if $P|_{S^n} = Q|_{S^n}$ then

$$P(x) = |x|^k P\left(\frac{x}{|x|}\right) = |x|^k Q\left(\frac{x}{|x|}\right) = Q(x)$$

which implies $P = Q$. ∎

Let $L^2(S^n)$ be the space of square integrable functions with an inner product given by

$$\langle f, g \rangle = \int_{S^n} fg \, d\sigma.$$

NB: if $P \in \mathcal{H}_k$ and $Q \in \mathcal{H}_j$ then

$$(k-j)\int_{S^n} PQ \, d\sigma = \int_{S^n} \left(Q \frac{\partial P}{\partial \nu} - P \frac{\partial Q}{\partial \nu} \right) d\sigma \quad \text{[by homogeneity]}$$

$$= \int_{B^n} (Q \Delta P - P \Delta Q) \, dx = 0$$

(i.e. the adjoint property)

Lemma. The set of finite linear combinations of elements in

$$\bigcup_{k=0}^{\infty} \mathcal{H}_k(S^n)$$

is (i) dense in $(C(S^n), \|\cdot\|_\infty)$, and
(ii) dense in $L^2(S^n)$.

(follows by an application of the Stone-Weierstrass thm)

Lemma. For every $P \in \mathcal{H}_k(n+1)$ the restriction $H = P|_{S^n} \in \mathcal{H}_k(S^n)$ is an eigenfunction of Δ_{S^n} for the eigenvalue $-k(n+k-1)$.

Proof. As $P(r\sigma) = r^k H(\sigma)$ for $r>0$, $\sigma \in S^n$, and

$$\boxed{\Delta f = \frac{1}{r^n}\frac{\partial}{\partial r}\left(r^n \frac{\partial f}{\partial r}\right) + \frac{1}{r^2}\Delta_{S^n} f}$$

we find that

$$\Delta P = \Delta(r^k H) = r^{k-2}\left(k(n+k-1)H + \Delta_{S^n} H\right).$$

Hence

$$\Delta P = 0 \iff \Delta_{S^n} H = -k(n+k-1)H. \qquad \blacksquare$$

Corollary. The spaces $\mathcal{H}_k(S^n)$ and $\mathcal{H}_l(S^n)$ are pairwise disjoint for $k \neq l$.

Theorem. (i) The eigenspaces of the Laplacian Δ_{S^n} are the spaces of spherical harmonics $\mathcal{H}_k(S^n)$ with corresponding eigenvalue $-k(n+k-1)$.

(ii) Each eigenspace representation is irreducible.

(iii) We have the Hilbert space direct sum decomposition

$$L^2(S^n) = \bigoplus_{k=0}^{\infty} \mathcal{H}_k(S^n),$$

i.e. the summands are closed pairwise orthogonal and every $f \in L^2(S^n)$ is the sum of an L^2-converging series of the form

$$f = \sum_{k=0}^{\infty} f_k,$$

where $f_k \in \mathcal{H}_k(S^n)$ are uniquely determined by f.

§ Spherical harmonics on the 2-sphere (†)

We want to find homogeneous polynomials of the form

$$P(r,\theta,\varphi) = r^l H(\theta,\varphi)$$

where $H = P|_{S^2} \in \mathcal{H}_l(S^2)$ that solve $\Delta P = 0$.

From the decomposition of the Laplacian, we have

$$\Delta P = 0 \iff \Delta_{S^2} H = -l(l+1)H. \qquad (*)$$

(i.e. H is an eigenfunction of Δ_{S^2} for the eigenvalue $-l(l+1)$.)

We can solve (∗) by the method of separation of variables:

if we suppose $H(\theta,\varphi) = \Theta(\theta)\Phi(\varphi)$ it follows that

$$\frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right) + l(l+1)\sin^2\theta = -\frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\varphi^2}$$

since

$$\Delta_{S^2} = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}.$$

(NB: the LHS is independent of the RHS)

This implies, for some constant μ, that

$$\begin{cases} \Phi'' + \mu\Phi = 0 \\ \dfrac{\sin\theta}{\Theta}\dfrac{\partial}{\partial\theta}\left(\sin\theta\dfrac{\partial\Theta}{\partial\theta}\right) + l(l+1)\sin^2\theta - \mu = 0 \end{cases}$$

(†) Here, using the convention: $\begin{cases} x = r\sin\theta\cos\varphi \\ y = r\sin\theta\sin\varphi \\ z = r\cos\theta \end{cases}$ $\quad 0 \le \theta \le \pi$, $0 \le \varphi \le 2\pi$

As Φ has to be periodic in φ, we require

$$\mu = m^2 \quad \text{for some } m \in \mathbb{N}_0 .$$

Then by solving $\Phi'' + m^2 \Phi = 0$ we get

$$\Phi(\varphi) = c_1 \cos m\varphi + c_2 \sin m\varphi .$$

On the other hand, we also have to solve

$$\sin^2\theta \, \Theta'' + \sin\theta \cos\theta \, \Theta' + \left(\ell(\ell+1)\sin^2\theta - m^2 \right) \Theta = 0 .$$

This equation is a variant of Legendre's equation. Using a change of variables, let $t = \cos\theta$, and consider

$$u(\cos\theta) = \Theta(\theta), \quad 0 \le \theta < \pi .$$

This yields the <u>general Legendre equation</u>:

$$(1-t^2)u'' - 2t u' + \left[\ell(\ell+1) - \frac{m^2}{1-t^2} \right] u = 0 .$$

The solution to this are given by the <u>associated Legendre polynomials</u>

$$u(t) = P_\ell^m(t) = (1-t^2)^{m/2} \frac{d^m}{dt^m} P_\ell(t) ,$$

where $P_\ell(t)$ are the <u>Legendre polynomials of the first kind</u>.

N.B.: $P_\ell^m = 0$ if $m > \ell$.

N.B.: $P_\ell(t) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{dt^\ell} (x^2-1)^\ell$ [Rodrigues' formula]

so that

$P_0(x) = 1$; $P_1(x) = x$; $P_2(x) = \frac{1}{2}(3x^2 - 1)$; etc...

We conclude the solutions $\Theta(\theta)$ are of the form

$$\Theta_{\ell m}(\theta) = \text{const.}\, P_\ell^m(\cos\theta) , \quad \ell > |m| ,$$

where we define $\Theta_{\ell,-|m|} = (-1)^m \Theta_{\ell,|m|}$.

Therefore the solutions $Y = \Theta \Phi$ are of the form(†)

$$Y_\ell^m(\theta, \varphi) = (-1)^m \sqrt{\frac{(2\ell+1)(\ell - |m|)!}{4\pi (\ell + |m|)!}} \, P_\ell^{|m|}(\cos\theta) \, e^{im\varphi}$$

for $m = -\ell, -\ell+1, \dots, \ell-1, \ell$. N.B.: $Y_{\ell m}^* = (-1)^m Y_{\ell,-m}$.

We say Y_ℓ^m are called <u>spherical harmonic functions of degree ℓ and order m</u>.

Here we have used the quantum mechanics normalization so that

$$\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta \, Y_\ell^m Y_{\ell'}^{m'} = \delta_{\ell\ell'} \delta_{mm'} .$$

N.B.:

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$Y_1^{-1} = \frac{1}{2}\sqrt{\frac{3}{2\pi}} e^{-i\varphi} \sin\theta = \frac{1}{2}\sqrt{\frac{3}{2\pi}} \left(\frac{x - iy}{r} \right)$$

$$Y_1^0 = \frac{1}{2}\sqrt{\frac{3}{\pi}} \cos\theta = \frac{1}{2}\sqrt{\frac{3}{\pi}} \frac{z}{r}$$

$$Y_1^1 = \frac{-1}{2}\sqrt{\frac{3}{2\pi}} e^{i\varphi} \sin\theta = \frac{-1}{2}\sqrt{\frac{3}{2\pi}} \frac{x + iy}{r}$$

where

$$\begin{cases} x = r \sin\theta \cos\varphi \\ y = r \sin\theta \sin\varphi \\ z = r \cos\theta \end{cases}$$

(†) Using the Condon-Shortley phase factor

§ Stationary Schrödinger's eqn. (separation of variables)

Consider a solution $\psi = \psi(\underline{r})$ to the PDE

$$\Delta\psi + 2\,(E - u(r))\,\psi = 0,$$

for a given potential $u = u(r)$ and a constant E (denoting the total energy).

As $\Delta\psi = \dfrac{\partial^2\psi}{\partial r^2} + \dfrac{2}{r}\dfrac{\partial\psi}{\partial r} + \dfrac{1}{r^2}\Delta_{S^2}\psi$

we suppose a solution is of the form

$$\boxed{\psi = R(r)\,Y(\theta, \varphi)}$$

This gives

$$\boxed{\frac{r^2}{R}\left(\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + 2(E - u(r))R\right) = \lambda = -\frac{1}{Y}\Delta_{S^2}Y}$$

NB: LHS $= f(r)$; RHS $= f(\theta, \varphi)$

Therefore $\lambda = \text{const}$.

Moreover the RHS equation $\Delta_{S^2}Y + \lambda Y = 0$ can be solved only if $\boxed{\lambda = \ell(\ell+1)}$, for $\ell = 0, 1, 2, \ldots$

We can then try solving the LHS equation

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \left[-\frac{\ell(\ell+1)}{r^2} + 2\,(E - u(r))\right]R = 0$$

by series expansion techniques.

NB: (1) For a Coulomb field $u(r) = -\dfrac{\alpha}{r}$, $\alpha > 0$, Bohr (1913) proposed discrete energy levels of the form

$$E = -\frac{\alpha}{2}\frac{1}{n^2}, \quad n = 1, 2, 3, \ldots$$

where n is the "principal quantum number".

(2) M. Born gave the interpretation $|\psi|^2 = \psi^*\psi$ = probability density.

(3) Normalised solutions $\psi = \psi_{n\ell m} = R_{n\ell}(r)\,Y_{\ell m}(\theta, \varphi)$ s.t. $\int|\psi|^2 = 1$ to

$$\begin{cases} \Delta_{S^2}Y + \ell(\ell+1)Y = 0 \\ \dfrac{d^2R}{dr^2} + \dfrac{2}{r}\dfrac{dR}{dr} - \dfrac{\ell(\ell+1)}{r^2}R + 2\left(-\dfrac{1}{2n^2} + \dfrac{1}{r}\right)R = 0 \end{cases}$$

have the following form:

(NB: $n = 1, 2, 3, 4, \ldots$; $\ell = 0, 1, 2, \ldots, n-1$; $m = -\ell, -\ell+1, \ldots, \ell-1, \ell$)

$$R_{n,l}[r] := \sqrt{\frac{(n-l-1)!}{(n+l)!}}\; e^{-\frac{r}{n}} \left(\frac{2r}{n}\right)^l \frac{2}{n^2}\,\text{LaguerreL}\left[n-l-1,\; 2l+1,\; \frac{2r}{n}\right]$$

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Y_{l,m}[θ, ϕ] := SphericalHarmonicY[l, m, θ, ϕ]
ψ_{n,l,m}[r, θ, ϕ] = R_{n,l}[r] Y_{l,m}[θ, ϕ]
Table[{{n, l, m}, ψ_{n,l,m}[r, θ, ϕ]^2}, {n, 1, 3}, {l, 0, n - 1}, {m, 0, l}]
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TableForm=

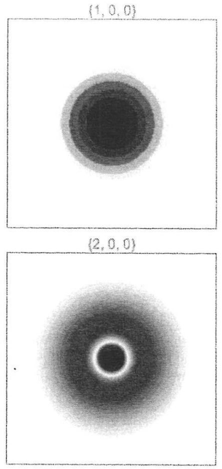
1 0 0	$\frac{e^{-2r}}{\pi}$				
2 0 0	$\frac{e^{-r}(-2+r)^2}{32\pi}$				
2 1 0	$\frac{e^{-r} r^2 \text{Abs}[\text{Cos}[\theta]]^2}{32\pi}$	2 1 1	$\frac{e^{-r} r^2 \text{Abs}[\text{Sin}[\theta]]^2}{64\pi}$		
3 0 0	$\frac{e^{-2r/3}(27-18r+2r^2)^2}{19683\pi}$				
3 1 0	$\frac{2e^{-2r/3}(-6+r)^2 r^2 \text{Abs}[\text{Cos}[\theta]]^2}{6561\pi}$	3 1 1	$\frac{e^{-2r/3}(-6+r)^2 r^2 \text{Abs}[\text{Sin}[\theta]]^2}{6561\pi}$		
3 2 0	$\frac{e^{-2r/3} r^4 \text{Abs}[1-3\text{Cos}[\theta]^2]^2}{39366\pi}$	3 2 1	$\frac{e^{-2r/3} r^4 \text{Abs}[\text{Cos}[\theta]\,\text{Sin}[\theta]]^2}{6561\pi}$	3 2 2	$\frac{e^{-2r/3} r^4 \text{Abs}[\text{Sin}[\theta]]^4}{26244\pi}$

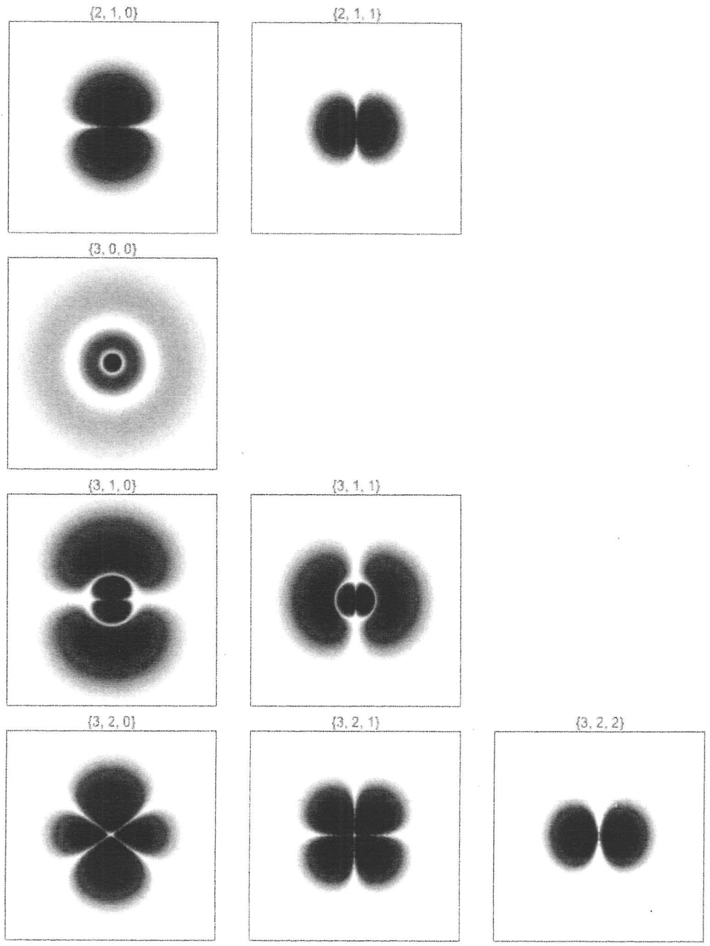
(Table of probability densities $|\psi|^2$ for $n = 1, 2, 3$)

NB: $dP = |\psi|^2 dx$ s.t. $\int dP = 1$.

Contour plots of $|\psi|^2$ in the plane $y=0$ for (n, ℓ, m).

NB: $\begin{bmatrix} \ell = 0, 1, \dots, n-1 \\ |m| = 0, 1, \dots, \ell-1 \end{bmatrix}$





Plots of $|Y_{\ell m}(\theta, \varphi)|^2$, NB: $|m| = 0, 1, \dots, \ell$.

Here $(x, y, z) = (r\sin\theta\cos\varphi,\ r\sin\theta\sin\varphi,\ r\cos\theta)$ for $0<\theta<\pi$, $0<\varphi<2\pi$

where $r = |Y_{\ell m}|^2$.