

Hydrogen atom

`SphericalHarmonicY[l, m, θ , ϕ]` gives the spherical harmonic $Y_l^m(\theta, \phi)$. It is the angular solution found in the Hydrogen atom.

Radial wave-function of the hydrogen atom:

$$\text{In[1]:= } \psi[n_, l_, m_, r_, \theta_, \phi_] := \sqrt{\frac{(n-l-1)!}{a^3 * (n+l)!}} e^{-\frac{r}{n*a}} \left(\frac{2 r}{n*a}\right)^l \\ \frac{2}{n^2} \text{LaguerreL}[n-l-1, 2l+1, \frac{2 r}{n*a}] * \text{SphericalHarmonicY}[l, m, \theta, \phi]$$

$$\text{In[2]:= } \psi[1, 0, 0, r, \theta, \phi]$$

$$\text{Out[2]= } \frac{\sqrt{\frac{1}{a^3}} e^{-\frac{r}{a}}}{\sqrt{\pi}}$$

$$\text{In[3]:= } \psi[2, 0, 0, r, \theta, \phi]$$

$$\text{Out[3]= } \frac{\sqrt{\frac{1}{a^3}} e^{-\frac{r}{2a}} \left(2 - \frac{r}{a}\right)}{4 \sqrt{2 \pi}}$$

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In[4]:= For[n = 1, n <= 3, n++,
  For[l = 0, l < n, l++,
    For[m = 0, m <= l, m++, Print["(n,l,m)->", n, l, m, " :  $\psi$ =",  $\psi[n, l, m, r, \theta, \phi]$ ]]]]

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$$(n, l, m) \rightarrow 100 : \psi = \frac{\sqrt{\frac{1}{a^3}} e^{-\frac{r}{a}}}{\sqrt{\pi}}$$

$$(n, l, m) \rightarrow 200 : \psi = \frac{\sqrt{\frac{1}{a^3}} e^{-\frac{r}{2a}} \left(2 - \frac{r}{a}\right)}{4 \sqrt{2 \pi}}$$

$$(n, l, m) \rightarrow 210 : \psi = \frac{\sqrt{\frac{1}{a^3}} e^{-\frac{r}{2a}} r \cos[\theta]}{4 a \sqrt{2 \pi}}$$

$$(n, l, m) \rightarrow 211 : \psi = -\frac{\sqrt{\frac{1}{a^3}} e^{-\frac{r}{2a} + i \phi} r \sin[\theta]}{8 a \sqrt{\pi}}$$

$$(n, l, m) \rightarrow 300 : \psi = \frac{\sqrt{\frac{1}{a^3}} e^{-\frac{r}{3a}} (27 a^2 - 18 a r + 2 r^2)}{81 a^2 \sqrt{3 \pi}}$$

$$(n, l, m) \rightarrow 310 : \psi = \frac{\sqrt{\frac{1}{a^3}} e^{-\frac{r}{3a}} r \left(4 - \frac{2r}{3a}\right) \cos[\theta]}{27 a \sqrt{2 \pi}}$$

$$(n, l, m) \rightarrow 311 : \psi = -\frac{\sqrt{\frac{1}{a^3}} e^{-\frac{r}{3a} + i \phi} r \left(4 - \frac{2r}{3a}\right) \sin[\theta]}{54 a \sqrt{\pi}}$$

$$(n, l, m) \rightarrow 320 : \psi = \frac{\sqrt{\frac{1}{a^3}} e^{-\frac{r}{3a}} r^2 (-1 + 3 \cos[\theta])^2}{81 a^2 \sqrt{6 \pi}}$$

$$(n, l, m) \rightarrow 321 : \psi = -\frac{\sqrt{\frac{1}{a^3}} e^{-\frac{r}{3a} + i \phi} r^2 \cos[\theta] \sin[\theta]}{81 a^2 \sqrt{\pi}}$$

$$(n, l, m) \rightarrow 322 : \psi = \frac{\sqrt{\frac{1}{a^3}} e^{-\frac{r}{3a} + 2 i \phi} r^2 \sin[\theta]^2}{162 a^2 \sqrt{\pi}}$$

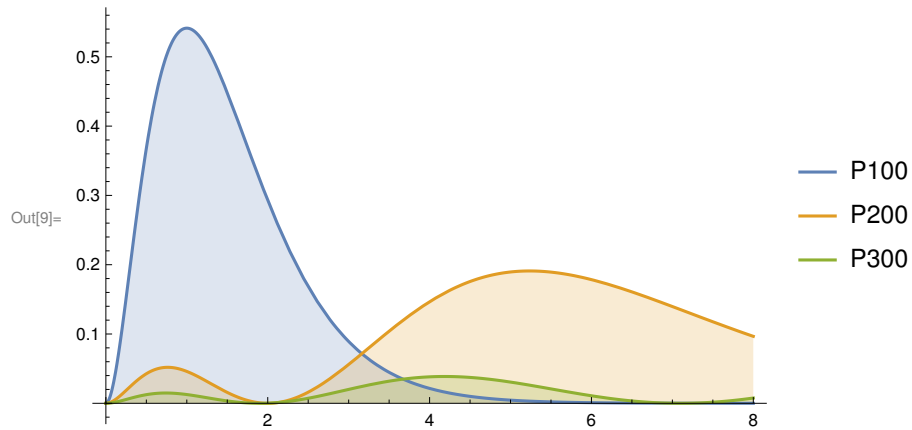
Probability density

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In[5]:= P[n_, l_, m_, r_, θ_, φ_] :=
  Simplify[4 π * r^2 * ψ[n, l, m, r, θ, φ] * Conjugate[ψ[n, l, m, r, θ, φ]],
    Element[{a, r}, Reals]] /. {a → 1}
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In[6]:= P100 = P[1, 0, 0, r,  $\theta$ ,  $\phi$ ];
P200 = P[2, 0, 0, r,  $\theta$ ,  $\phi$ ];
P300 = P[3, 0, 0, r,  $\theta$ ,  $\phi$ ];
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Out[6]= $4 e^{-2 r} r^2$

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In[9]:= Plot[{P100, P200, P300}, {r, 0, 8}, PlotLegends → "Expressions", Filling → Bottom]
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In[10]:= Plot[{P100, P200, P300}, {r, 0, 20}, PlotLegends → "Expressions"]
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