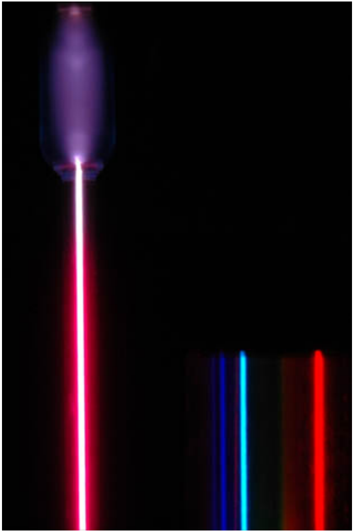
What is this?



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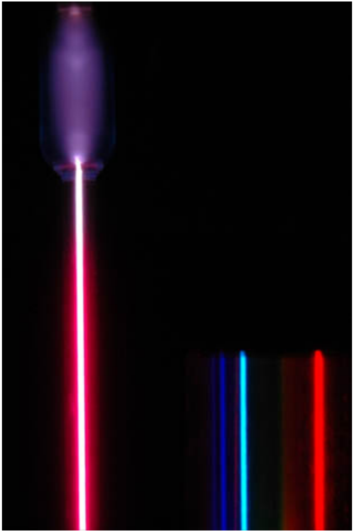

The Hydrogen Atom

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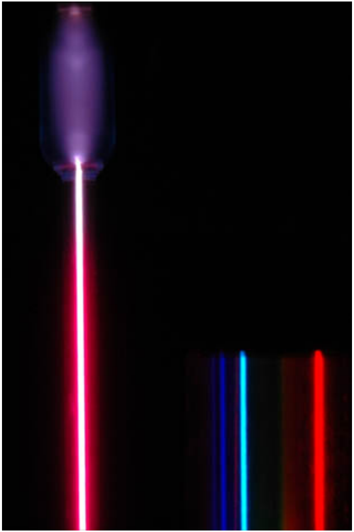
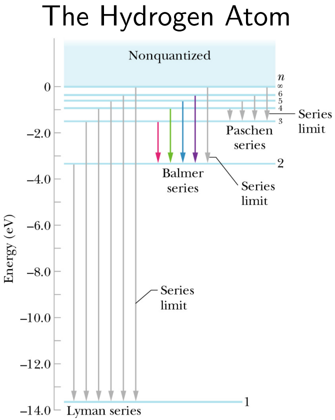
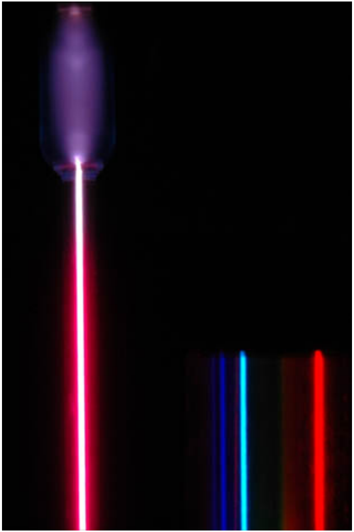




The Hydrogen Atom
Nonquantized
n
∞
6
5
4
3
2
1
Series limit
Paschen series
Balmer series
Series limit
Series limit
Lyman series
Energy (eV)
0
–2.0
–4.0
–6.0
–8.0
–10.0
–12.0
–14.0

What is this?



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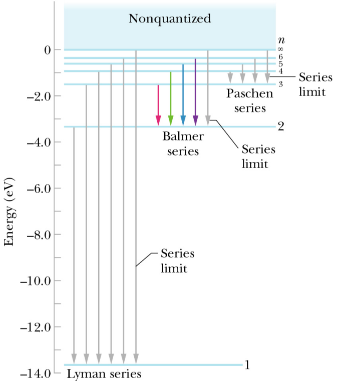

$$\frac{1}{\lambda} = R_H \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

R_H - Rydberg constant

Hydrogen Eigenvalues

$$E_n = -\frac{13.6\ eV}{n^2}$$

Quantitative comparison for Balmer series hydrogen in units of σ.

Line	My Results (Å)	NIST Results (Å)	Normalized Difference	Percent Difference
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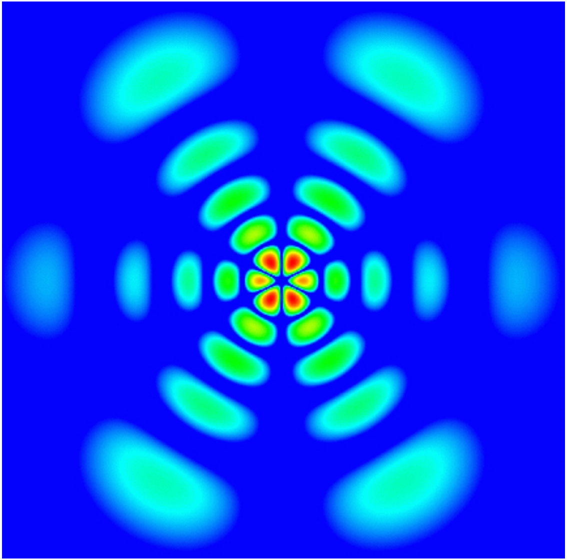
$n = 8,\ l = 3,\ m = 1$



How do we build the quantum model?

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$$E = \frac{p^2}{2\mu} - \frac{e^2}{r} = \frac{p_r^2}{2\mu} + \frac{L^2}{2\mu r^2} - \frac{e^2}{r} \qquad \mu = \frac{m_p m_e}{m_p + m_e} \approx m_e$$

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$$-\frac{\hbar^2}{2\mu}\left(\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial^2\phi}\right)\varphi_s(\vec{r}) - \frac{e^2}{r}\varphi_s(\vec{r}) = E\varphi_s(\vec{r})$$

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GO SOLVE IT!

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Hydrogen Bound State Eigenfunctions

$$\begin{aligned}\varphi_{nlm}(r,\theta,\phi) &= R_{nl}(r)Y_l^m(\theta,\phi) \\ &= (2\kappa)^{3/2} A_{nl}\rho^l e^{-\rho/2} F_{nl}(\rho) Y_l^m(\theta,\phi)\end{aligned}$$

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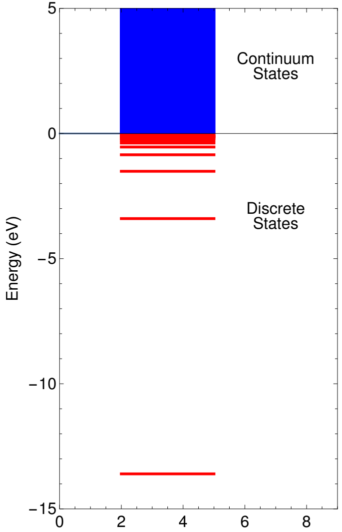
$$F(\rho) = \sum_{i=0}^{\infty} = a_i\rho^i \Rightarrow a_{i+1} = \frac{(i+l+1)-\lambda}{(i+1)(i+2l+2)}a_i \quad a_0 = 1$$

$$E_n = -|E| \quad \rho = 2\kappa r \quad \kappa = \sqrt{\frac{2\mu|E|}{\hbar^2}} \quad \lambda = \frac{Ze^2}{\hbar}\sqrt{\frac{\mu}{2|E|}}$$

$$F_{nl}(\rho) = L_{n-l-1}^{2l+1}(\rho) \quad A_{nl} = \sqrt{\frac{(n-l-1)!}{2n[(n+l)!]^3}}$$

Hydrogen Eigenvalues (Energy Levels)

$$E_n = -\frac{\mu(e^2)^2}{2\hbar^2 n^2} = -\frac{13.6\ eV}{n^2}$$



Hydrogen Bound State Eigenfunctions

$$\begin{aligned}\psi_{Enlm}(r,\theta,\phi) &= R_{nl}(r)Y_l^m(\theta,\phi)\\ &= A_{nl}\rho^l e^{-\rho}\left(\sum_{k=0}^{k_{max}} b_k\rho^k\right)Y_l^m(\theta,\phi)\end{aligned}$$

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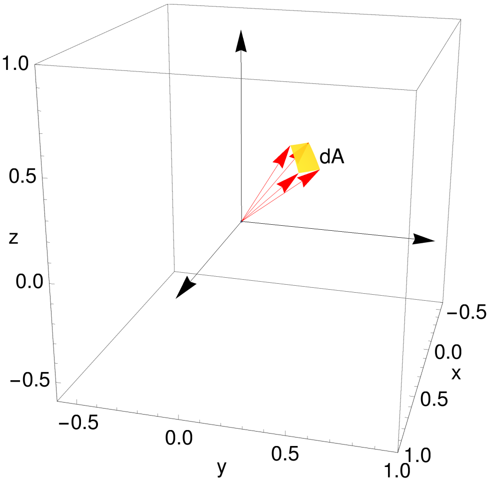
$$= A_{nl}\rho^l e^{-\rho}\left(\sum_{k=0}^{k_{max}} b_k \rho^k\right) Y_l^m(\theta,\phi)$$

$$b_{k+1} = \frac{2(k+l+1)-\lambda e^2}{(k+1)(k+2l+2)} b_k \quad b_0 = 1$$

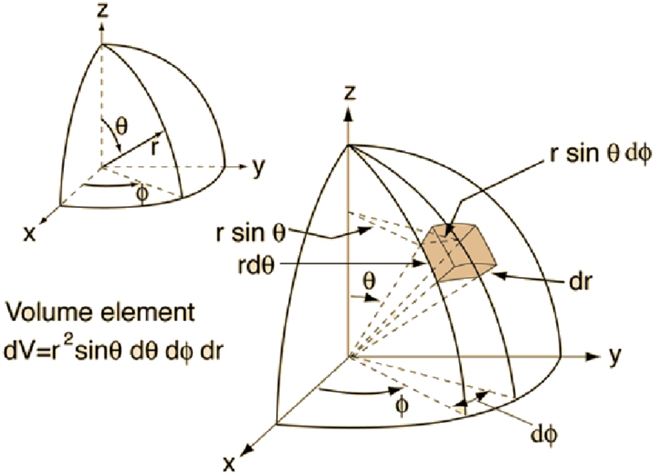
$$E_n = -W \quad \rho = \kappa r \quad \kappa = \sqrt{\frac{2\mu W}{\hbar^2}} \quad \lambda = \sqrt{\frac{2\mu}{\hbar^2 W}} \quad a_0 = \frac{\hbar^2}{me^2}$$

$$\psi_{Enlm} = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}}\; e^{-r/na_0}\left(\frac{2r}{na_0}\right)^l (n+l)!\; \mathcal{L}_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right) Y_l^m(\theta,\phi)$$

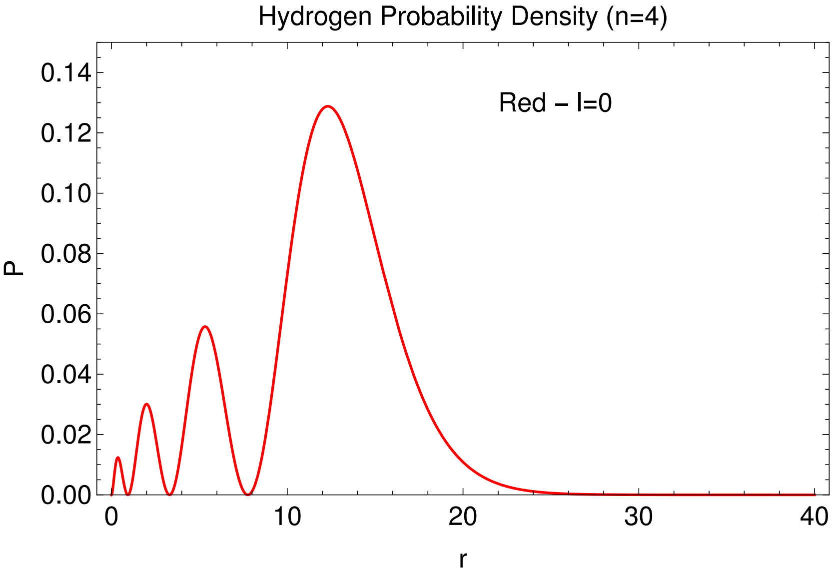
Recall the Solid Angle



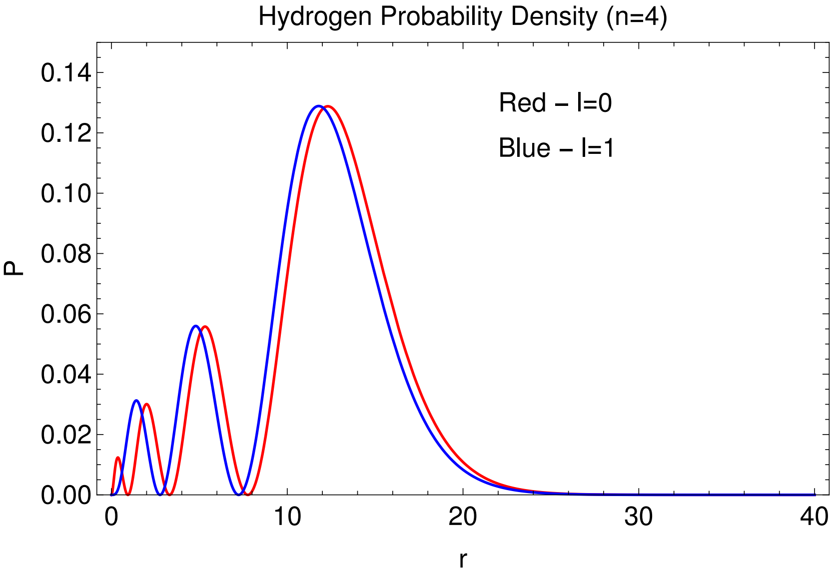
Spherical Differential Volume Element



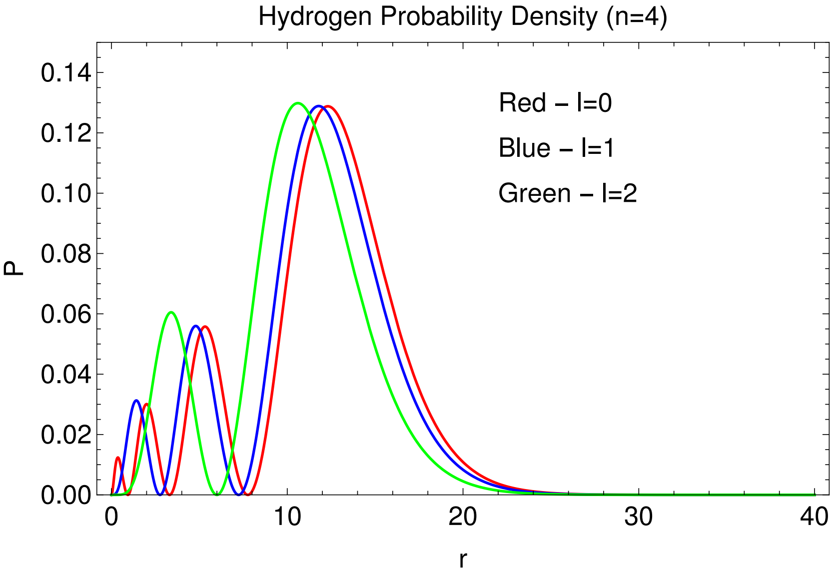
Hydrogen Eigenfunctions



Hydrogen Eigenfunctions



Hydrogen Eigenfunctions



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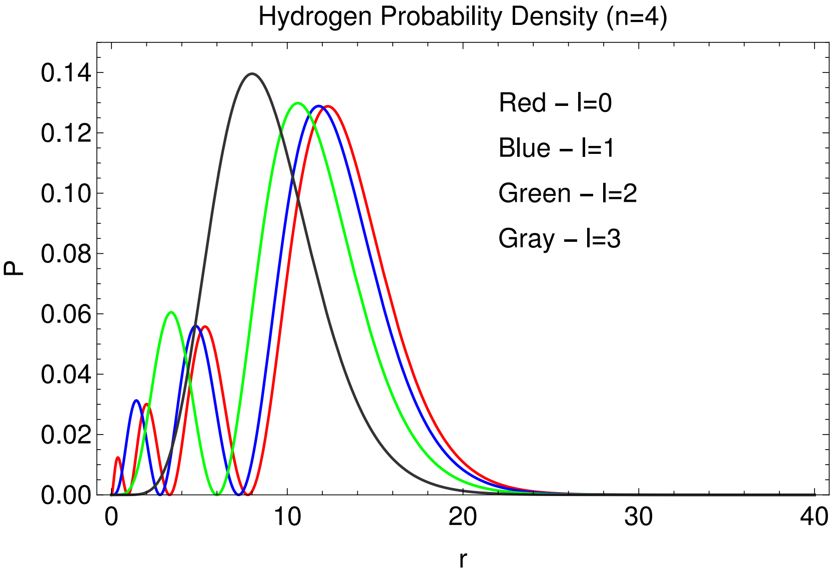
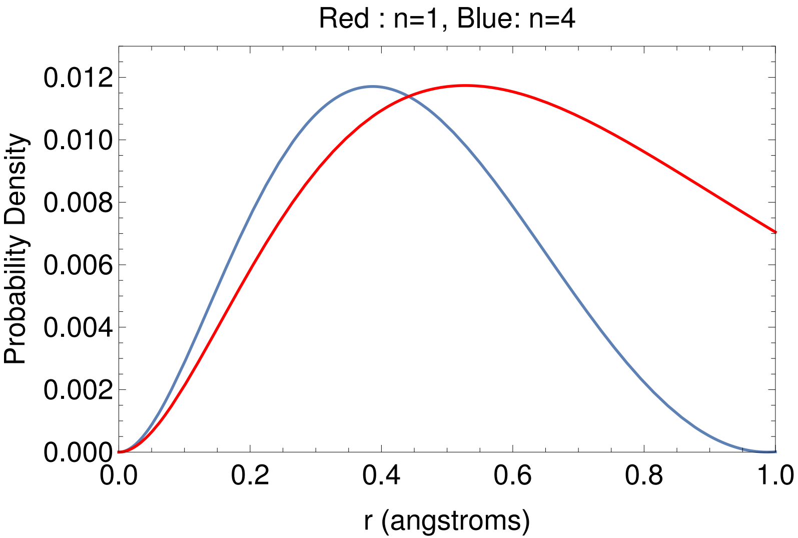


Do the peaks line up?



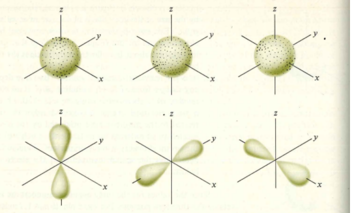


FIGURE 5-10

Location Probability Patterns for the *p* Orbitals

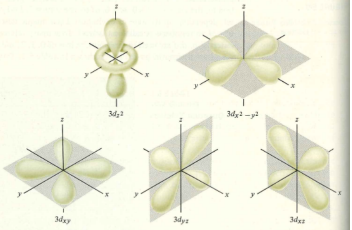
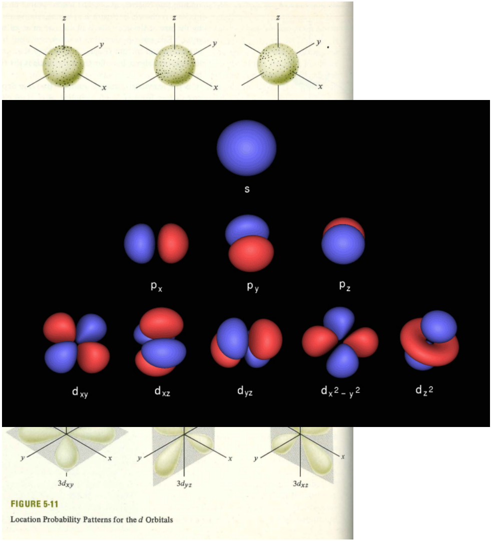


FIGURE 5-11

Location Probability Patterns for the *d* Orbitals

Old Orbitals - New Orbitals



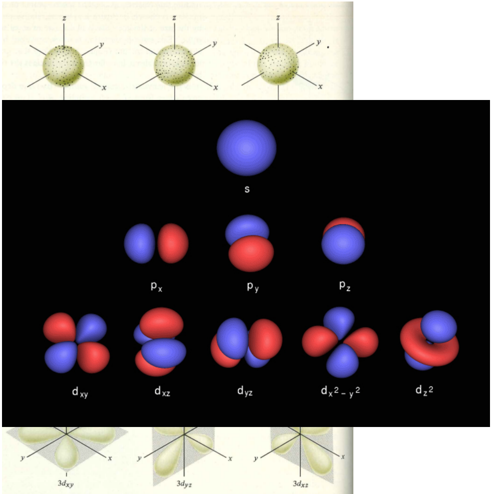
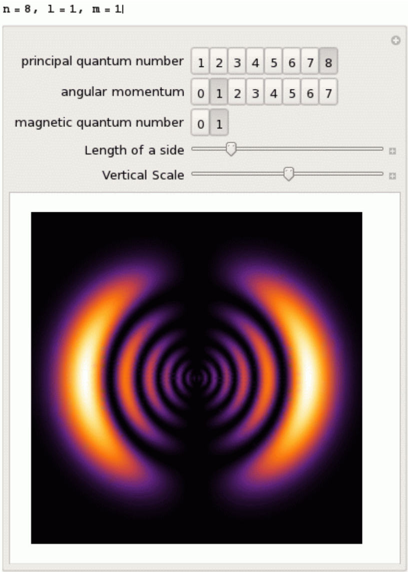


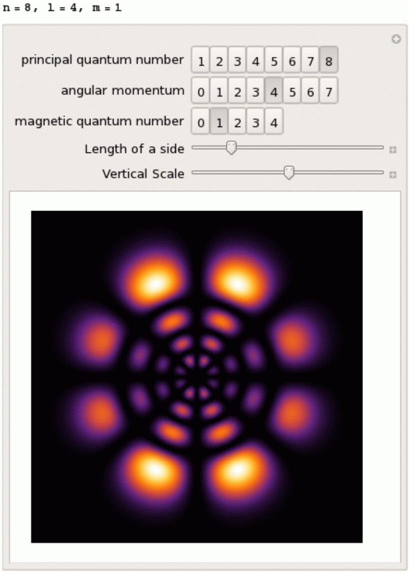
FIGURE 5-11

Location Probability Patterns for the *d* Orbitals

How are these plots related to what we know?

More Hydrogen Eigenfunctions





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Quantitative comparison for Balmer series hydrogen in units of σ.

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$$\alpha : n = 3 \rightarrow n = 2$$

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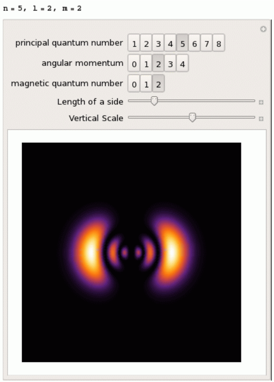
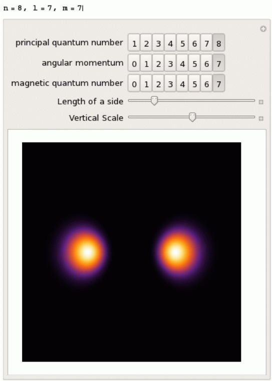
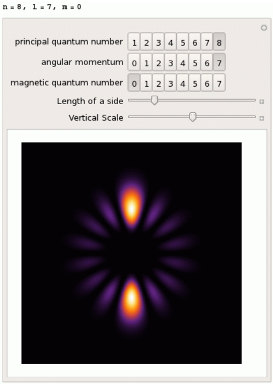
Some Plots


n = 5, l = 2, m = 2
principal quantum number 1 2 3 4 5 6 7 8
angular momentum 0 1 2 3 4
magnetic quantum number 0 1 2
Length of a side
Vertical Scale


n = 8, l = 7, m = 7
principal quantum number 1 2 3 4 5 6 7 8
angular momentum 0 1 2 3 4 5 6 7
magnetic quantum number 0 1 2 3 4 5 6 7
Length of a side
Vertical Scale


n = 8, l = 7, m = 0
principal quantum number 1 2 3 4 5 6 7 8
angular momentum 0 1 2 3 4 5 6 7
magnetic quantum number 0 1 2 3 4 5 6 7
Length of a side
Vertical Scale