Problem Set 11

Hydrogen Atom

1. Show that the hydrogen atom ψ_{n,l,m_l} wavefunctions are eigenfunctions of the Hamiltonian.
2. Determine whether or not the hydrogen atom ψ_{n,l,m_l} wavefunctions are eigenfunctions of the $\hat{L}_z$ operator. What are the eigenvalues?
3. Determine whether or not the hydrogen atom ψ_{n,l,m_l} wavefunctions are eigenfunctions of the $\hat{L}^2$ operator. What are the eigenvalues?
4. Show that the ψ_{n,l,m_l} wavefunctions are orthonormal.
5. Calculate the expectation value: $\langle \hat{r} \rangle$, where $\hat{r} = r$ for the ψ_{n,l,m_l} wavefunctions.
6. Calculate the expectation value: $\langle \hat{x} \rangle$, where $\hat{x} = r \sin\theta \cos\phi$ for the ψ_{n,l,m_l} wavefunctions.
7. Calculate the expectation value: $\langle \hat{y} \rangle$, where $\hat{y} = r \sin\theta \sin\phi$ for the ψ_{n,l,m_l} wavefunctions.
8. Calculate the expectation value: $\langle \hat{z} \rangle$, where $\hat{z} = r \cos\theta$ for the ψ_{n,l,m_l} wavefunctions.
9. Plot the radial part of the hydrogen atom wavefunction, $R_{n,l}$, for the lowest few values of n and l.

Some Potentially Useful Equations

Hydrogen Atom

$\psi_{n,l,m_l}(r,\theta,\phi) = R_{n,l}(r)Y_{l,m_l}(\theta,\phi)$

$E_n = -\frac{me^4}{2\hbar^2(4\pi\epsilon_0)^2}\frac{1}{n^2}$

$a = \frac{4\pi\epsilon_0\hbar^2}{me^2}$

$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$

$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right)$

$Y_{0,0} = \left(\frac{1}{4\pi}\right)^{1/2}$

$Y_{1,0} = \left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$

$Y_{1,\pm1} = \mp\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta\ \mathrm{e}^{\pm i\phi}$

$Y_{2,0} = \left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta - 1)$

$Y_{2,\pm1} = \mp\left(\frac{15}{8\pi}\right)^{1/2}\cos\theta\sin\theta\ \mathrm{e}^{\pm i\phi}$

$Y_{2,\pm2} = \left(\frac{15}{32\pi}\right)^{1/2}\sin^2\theta\ \mathrm{e}^{\pm 2i\phi}$

$R_{1,0} = 2a^{-3/2}e^{-r/a}$

$R_{2,0} = \frac{1}{\sqrt{2}}a^{-3/2}\left(1 - \frac{r}{2a}\right)e^{-r/2a}$

$R_{2,1} = \frac{1}{\sqrt{24}}a^{-3/2}\left(\frac{r}{a}\right)e^{-r/2a}$

$R_{3,0} = \frac{2}{\sqrt{27}}a^{-3/2}\left(1 - \frac{2r}{3a} + \frac{2r^2}{27a^2}\right)e^{-r/3a}$

$R_{3,1} = \frac{8}{27\sqrt{6}}a^{-3/2}\left(\frac{r}{a} + \frac{r^2}{6a^2}\right)e^{-r/3a}$

$R_{3,2} = \frac{4}{81\sqrt{30}}a^{-3/2}\left(\frac{r^2}{a^2}\right)e^{-r/3a}$

Angular momentum operators

$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) = -i\hbar\left(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$

$\hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) = -i\hbar\left(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$

$\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\left(\frac{\partial}{\partial\phi}\right)$

$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$

Spherical Polar Coordinates

$x = r\sin\theta\cos\phi$

$y = r\sin\theta\sin\phi$

$z = r\cos\theta$

$\int_{x=-\infty}^{\infty}\int_{y=-\infty}^{\infty}\int_{z=-\infty}^{\infty} f(x,y,z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z \equiv \int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi}\int_{r=0}^{\infty} f(r,\theta,\phi)\sin\theta\, r^2\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi$