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1. Using tables of the spherical harmonics ($Y_{l,m_l}(\theta,\phi)$) and associated Laguerre fybctions, which respectively form the angular ($Y_{l,m_l}(\theta,\phi)$) and radial ($R_{nl}(r)$) components of the hydrogen atom wavefunction, write down the form of the 2p$_\mathrm{x}$ orbital (Hint: Write down the $m_s = -1$ 2p orbital, use the Euler relation, and take the real component which can be obtained from $\frac{1}{2}(\psi_{-1} + \psi^*_{-1})$, then realize in spherical polar coordinates, $x = r\cos\phi\sin\theta$).

Using the fact that $r = \sqrt{x^2+y^2+z^2}$ and setting any constants equal to one, plot a contour plot of the 2p$_\mathrm{x}$ orbital (Hint: go to emphhttps://www.wolframalpha.com/ and add "*contour plot of x*e ^(-sqrt(x ^2+y ^2)/2), x=-8..8, y=-8..8*" to the entry line and press enter).

$\psi_{2,1,-1} = \frac{1}{(16\pi a_0^5)^{1/2}} r\sin(\theta)e^{-i\phi}e^{-r/2a_0}$

$\psi_{2,1,-1} = \frac{1}{(16\pi a_0^5)^{1/2}} r\sin(\theta)\{\cos(\phi) - i\sin(\phi)\}e^{-r/2a_0}$

$\psi_{2,1,Re(-1)} = \frac{1}{2}\big(\psi_{2,1,-1} + \psi^*_{2,1,-1}\big) = \big(\frac{1}{(16\pi a_0^5)^{1/2}} r\sin(\theta)\cos(\phi)e^{-r/2a_0}$

$\psi_{2,1,Re(-1)} = \frac{1}{(16\pi a_0^5)^{1/2}} xe^{-r/2a_0}$

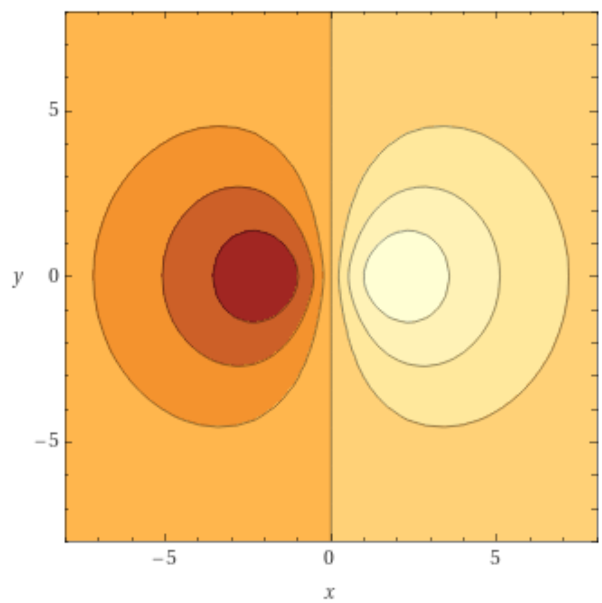

Figure 1: 2p$_\mathrm{x}$ orbital from Wolfram Alpha plot

2. Determine the probability that an electron in a hydrogen 1s orbital will be found at $r = 1.8$ a$_0$ distance from the nucleus given the radial distribution function $P(r) = R(r)^2r^2$.

$P(r) = r^2R(r)^2 = r^2\big\{2\big(\frac{1}{a_0}\big)^{\frac{3}{2}}\exp(-r/a_0)\big\}^2 = r^2\big(\frac{4}{a_0^3}\big)\exp(-2r/a_0)$

$P(1.8a_0) = 1.8^2a_0^2\big(\frac{4}{a_0^3}\big)\exp(-2\times 1.8a_0/a_0) = \big(\frac{12.96}{a_0}\big)\exp(-3.6) = 0.354a_0^{-1}$

3. Determine the average distance of the electron from the nucleus in a hydrogen 1s orbital (*Hint*: compute the expectation value of $\hat{r}$ by integrating over both angular and radial terms where $d\tau = r^2dr\sin(\theta)d\theta d\phi$).

$\langle \hat{r} \rangle = \frac{\langle \psi_{1,0,0} | \hat{r} | \psi_{1,0,0} \rangle}{\langle \psi_{1,0,0} | \psi_{1,0,0} \rangle}$
Using the normalization of the wavefunction
$\langle \hat{r} \rangle = \langle \psi_{1,0,0} | \hat{r} | \psi_{1,0,0} \rangle = \int \psi^*_{1,0,0} r \psi_{1,0,0} d\tau = \int_0^\infty \int_0^\pi \int_0^{2\pi} \psi^*_{1,0,0} r \psi_{1,0,0} r^2 dr \sin(\theta) d\theta d\phi$
Using the fact that the angular part is square integrable to 1
$\langle \hat{r} \rangle = \int_0^\infty R_{1,0}(r)^* r R_{1,0}(r)^* r^2 dr = \int_0^\infty R_{1,0}(r)^2 r^3 dr = \int_0^\infty \left(\frac{4}{a_0^3}\right) \exp(-2r/a_0) r^3 dr$
Integration by parts is the easiest route (we have to do it three times recursively until we have an integral of just the exponential function), setting $f = r^3$ and $g' = e^{-2r/a_0}$ and so on we get $\langle \hat{r} \rangle = [\frac{-2}{a_0^2} r^3 e^{-2r/a_0} - \frac{3}{a_0} r^2 e^{-2r/a_0} - 3re^{-2r/a_0} - \frac{3a_0}{2} e^{-2r/a_0}]_0^\infty = \frac{3a_0}{2}$

4. A potential is applied to a particle in a one-dimensional box of $V = -\epsilon \sin\left(\frac{\pi x}{L}\right)$. Determine the first-order correction to the ground state energy using perturbation theory (*Hint:* $\sin^3(x) = \frac{1}{4}\{3\sin(x) - \sin(3x)\}$).

$\psi_1^{(0)} = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L} x\right)$
$\hat{H}^{(1)} = -\varepsilon \sin\left(\frac{\pi x}{L}\right)$
$E_1^{(1)} = \int_0^L \psi_1^{(0)^*} \hat{H}^{(1)} \psi_1^{(0)} dx = -\frac{2\varepsilon}{L} \int_0^L \sin^3\left(\frac{\pi}{L} x\right) dx = -\frac{3\varepsilon}{2L} \int_0^L \sin\left(\frac{\pi}{L} x\right) + \frac{\varepsilon}{2L} \int_0^L \sin\left(\frac{3\pi}{L} x\right) dx$
$E_1^{(1)} = \left[\left(\frac{3\varepsilon}{2L}\right) \cos\left(\frac{\pi}{L} x\right) \left(\frac{L}{\pi}\right)\right]_0^L + \left[-\left(\frac{\varepsilon}{2L}\right) \cos\left(\frac{3\pi}{L} x\right) \left(\frac{L}{3\pi}\right)\right]_0^L$
$E_1^{(1)} = \left(\frac{3\varepsilon}{2L}\right) \cos(\pi) \left(\frac{L}{\pi}\right) - \left(\frac{3\varepsilon}{2L}\right) \cos(0) \left(\frac{L}{\pi}\right) - \left(\frac{\varepsilon}{2L}\right) \cos(3\pi) \left(\frac{L}{3\pi}\right) + \left(\frac{\varepsilon}{2L}\right) \cos(0) \left(\frac{L}{3\pi}\right)$
$E_1^{(1)} = -\left(\frac{3\varepsilon}{2L}\right)\left(\frac{L}{\pi}\right) - \left(\frac{3\varepsilon}{2L}\right)\left(\frac{L}{\pi}\right) + \left(\frac{\varepsilon}{2L}\right)\left(\frac{L}{3\pi}\right) + \left(\frac{\varepsilon}{2L}\right)\left(\frac{L}{3\pi}\right)$
$E_1^{(1)} = -\frac{8\varepsilon}{3\pi}$