Assignment 12

1) $\Psi_{3p_0}\{\vec{r}\} = \sqrt{\frac{2}{3^8\pi}} \cdot (r) \cdot (6-r) e^{-r/3} \cos\theta$

a) roots: $R_{3p_0}\{\vec{r}\} = 0 = \sqrt{\frac{2}{3^8\pi}}\, r(6-r)e^{-r/3}$

$0 = r(6-r)(e^{-r/3})$

$r = 0 \quad 6-r=0 \quad e^{-r/3} \neq 0$

$r=0 \quad r=6$

máx + min:

$\frac{\partial R}{\partial r} = 0 = \sqrt{\frac{2}{3^8\pi}}\left[(6-r)e^{-r/3} - re^{-r/3} - \frac{1}{3}r(6-r)e^{-r/3}\right]$

$0 = e^{-r/3}\left[(6-r) - r - \frac{1}{3}(6r - r^2)\right]$

$e^{-r/3} \neq 0 \qquad 0 = 6 - 2r - 2r + r^2/3$

$\frac{r^2}{3} - 4r + 6 = 0$

$r = \frac{4 \pm \sqrt{16-8}}{(2/3)} = \frac{3(4 \pm 2\sqrt{2})}{2} = 3(2 \pm \sqrt{2})$

$\approx (8.83,\ 3.17)$

b) $P\{r\} = \int_0^{\pi} d\theta \int_0^{2\pi} d\phi \left[|\Psi\{r,\theta,\phi\}|^2 r^2 \sin\theta\right] = \int_0^{\pi} d\theta \int_0^{2\pi} d\phi \left[\left|\sqrt{\frac{2}{3^8\pi}}\, r(6-r)e^{-r/3}\cos\theta\right|^2 r^2 \sin\theta\right]$

$= 2\pi\left(\int_0^{\pi} |\cos\theta|^2 \sin\theta\, d\theta\right)\left(\frac{2}{3^8\pi}\right)|r|^2|6-r|^2|e^{-r/3}|^2 r^2 = 2\pi\left(\frac{2}{3^8\pi}\right)\left(\frac{2}{3}\right)|r|^2|6-r|^2|e^{-r/3}|^2 r^2$

cosθ always real so $\longrightarrow \int_0^{\pi} \cos\theta^2 \sin\theta\, d\theta = -\int_0^{\pi} u^2\, du = -\frac{u^3}{3}\Big|_0^{\pi} = -\left(\frac{\cos^3\theta}{3}\right)\Big|_0^{\pi} = -\left(\frac{-1^3}{3}\right) + \left(\frac{1^3}{3}\right) = \frac{2}{3}$

$= \frac{2^3}{3^9}|r|^2|6-r|^2|e^{-r/3}|^2 r^2 \xrightarrow{r \text{ is real}} = \frac{2^3}{3^9} r^4 (6-r)^2 e^{-2r/3}$

c) roots: $P\{r\} = 0 \longrightarrow r = 0$ or $r = 6$

$\frac{dP}{dr} = 0 = \frac{d}{dr}\left[r^4(6-r)^2 e^{-2r/3}\right] = \frac{d}{dr}\left[r^4(36 - 12r + r^2)e^{-2r/3}\right] = \frac{d}{dr}\left[e^{-2r/3}(36r^4 - 12r^5 + r^6)\right]$

$0 = -\frac{2}{3}e^{-2r/3}(36r^4 - 12r^5 + r^6) + e^{-2r/3}(144r^3 - 60r^4 + 6r^5)$

$0 = e^{-2r/3}\left[-24r^4 + 8r^5 - \frac{2}{3}r^6 + 144r^3 - 60r^4 + 6r^5\right]$

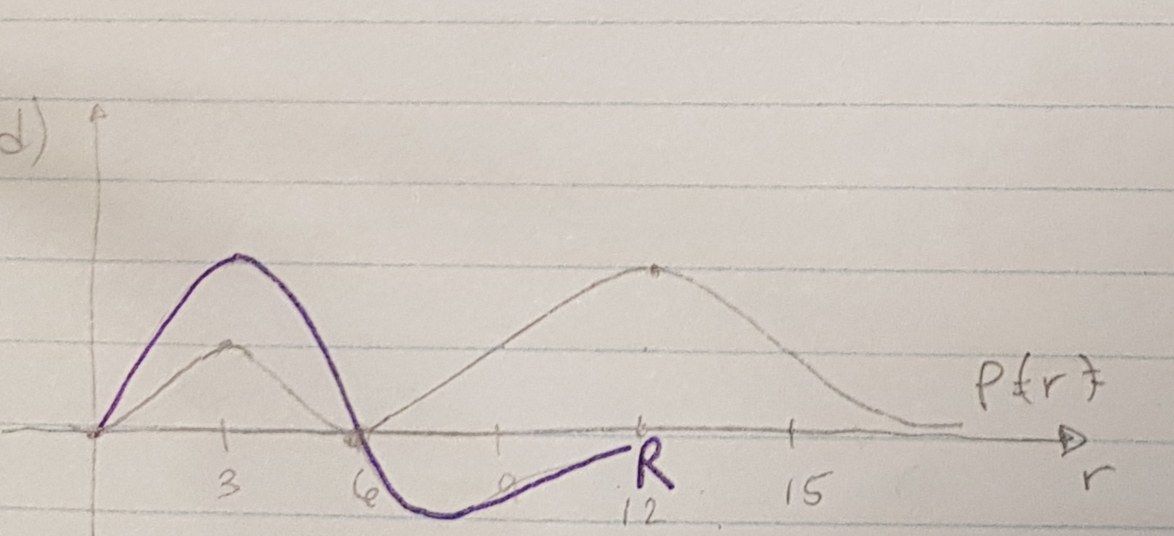
$0 = e^{-2r/3}\left[144r^3 - 84r^4 + 14r^5 - \frac{2}{3}r^6\right] = \underbrace{e^{-2r/3}}_{\neq 0}\ \underbrace{r^3}_{r=0}\ \underbrace{\left(144 - 84r + 14r^2 - \frac{2}{3}r^3\right)}_{r=0}$

$0 = 144 - 84r + 14r^2 - \frac{2}{3}r^3$

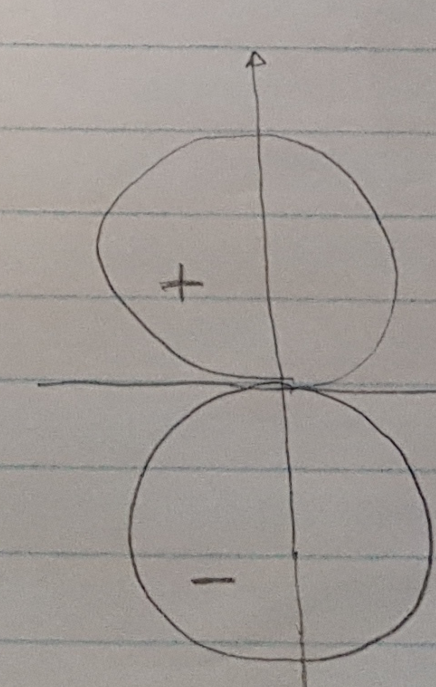
$r = 3, 6, 12$

min + máx: $r = 0, 3, 6, 12$

d)



e)



$Y_{3p_0} = \cos\theta$

2) $[\hat{L}_x, \hat{L}_y]f = (\hat{L}_x\hat{L}_y f - \hat{L}_y\hat{L}_x f) = -\hbar^2\left[\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\left(z\frac{\partial f}{\partial x} - x\frac{\partial f}{\partial z}\right) - \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\left(y\frac{\partial f}{\partial z} - z\frac{\partial f}{\partial y}\right)\right]$

$= -\hbar^2\left[y\frac{\partial f}{\partial x} + yz\frac{\partial^2 f}{\partial x \partial z} - z^2\frac{\partial^2 f}{\partial x \partial y} + xz\frac{\partial^2 f}{\partial y \partial z} - yz\frac{\partial^2 f}{\partial x \partial z} + z^2\frac{\partial^2 f}{\partial x \partial y} + xy\frac{\partial^2 f}{\partial z^2} - x\frac{\partial f}{\partial y} - xz\frac{\partial^2 f}{\partial y \partial z} - xy\frac{\partial^2 f}{\partial z^2}\right]$

$= -\hbar^2\left[y\frac{\partial f}{\partial x} - x\frac{\partial f}{\partial y}\right] = \hbar^2\left[x\frac{\partial f}{\partial y} - y\frac{\partial f}{\partial x}\right] = i\hbar\hat{L}_z f$

$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$; $[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x$, $[\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$

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

$= \hat{L}_y\hat{L}_y\hat{L}_x - \hat{L}_x\hat{L}_y\hat{L}_y + \hat{L}_z\hat{L}_z\hat{L}_x - \hat{L}_x\hat{L}_z\hat{L}_z$

$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z \qquad [\hat{L}_y, \hat{L}_x] = -i\hbar\hat{L}_z$

$\hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x = i\hbar\hat{L}_z \qquad \hat{L}_y\hat{L}_x - \hat{L}_x\hat{L}_y = -i\hbar\hat{L}_z$

$\hat{L}_y\hat{L}_x = \hat{L}_x\hat{L}_y - i\hbar\hat{L}_z \qquad \hat{L}_x\hat{L}_y\hat{L}_y = \hat{L}_y\hat{L}_x\hat{L}_y + i\hbar\hat{L}_z\hat{L}_y$

$\hat{L}_y\hat{L}_y\hat{L}_x = \hat{L}_y\hat{L}_x\hat{L}_y - i\hbar\hat{L}_y\hat{L}_z$

$= \hat{L}_y\hat{L}_x\hat{L}_y - i\hbar\hat{L}_y\hat{L}_z - \hat{L}_y\hat{L}_x\hat{L}_y + i\hbar\hat{L}_z\hat{L}_y + \hat{L}_z\hat{L}_z\hat{L}_x - \hat{L}_x\hat{L}_z\hat{L}_z$

$[\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$

$\hat{L}_z\hat{L}_x - \hat{L}_x\hat{L}_z = i\hbar\hat{L}_y \qquad \hat{L}_x\hat{L}_z = \hat{L}_z\hat{L}_x - i\hbar\hat{L}_y$

$\hat{L}_z\hat{L}_z\hat{L}_x = \hat{L}_z\hat{L}_x\hat{L}_z + i\hbar\hat{L}_z\hat{L}_y \qquad \hat{L}_x\hat{L}_z\hat{L}_z = \hat{L}_z\hat{L}_x\hat{L}_z - i\hbar\hat{L}_y\hat{L}_z$

$= -i\hbar\hat{L}_y\hat{L}_z + i\hbar\hat{L}_z\hat{L}_y + \hat{L}_z\hat{L}_x\hat{L}_z + i\hbar\hat{L}_z\hat{L}_y - \hat{L}_z\hat{L}_x\hat{L}_z + i\hbar\hat{L}_y\hat{L}_z = 0$

$[\hat{L}^2, L_y] = 0$, $[\hat{L}^2, L_z] = 0$

3) $E\{\zeta\} = -\zeta^2 + \frac{5}{8}\zeta + 2\zeta^2 - 2\zeta Z$

$\frac{\partial E}{\partial \zeta} = 0 = -2\zeta + \frac{5}{8} + 4\zeta - 2Z$

$\zeta = \frac{2Z - 5/8}{2}$

$\zeta = Z - 5/16$

$E\{Z - 5/16\} = -(Z - 5/16)^2 + \frac{5}{8}(Z - 5/16) + 2(Z - 5/16)^2 - 2(Z - 5/16)Z = -(Z - 5/16)^2$

$\zeta_{He} = 2 - 5/16 = 1.6875$

$E_{He}\{\zeta\} = -2.848$ Hartree

4) $E_n = \frac{Z^2}{2n^2}$ {a.u}

$\Delta E = E_{n_i} - E_{n_f} = \frac{Z^2}{2}\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right) = \frac{hc}{\lambda_{vac}}$

$\frac{1}{\lambda_{vac}} = \frac{Z^2}{2hc}\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$

$\frac{1}{2hc}$ Hartree $(4.35974 \times 10^{-18}\ \text{J/Hartree}) = 1.09737 \times 10^{7}\ \text{m}^{-1} = R$

$\frac{1}{\lambda_{vac}} = RZ^2\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$

$n_i > n_f \rightarrow$ Not a negative wavelength, this just means that the photon was emitted instead of absorbed.