Hooray, Last Homework! (HW 13)

4.52. S.E: $i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2M} \nabla^2 \Psi + V\Psi$; For $\Psi(r,\phi,t) = R(r)P(\phi)T(t)$

$\Rightarrow$ Separation of variables:
$$\left.\begin{aligned} i\hbar \frac{T'(t)}{T(t)} &= E \quad (1) \\ -\frac{P''(\phi)}{P(\phi)} &= F \quad (2) \\ \frac{r}{R(r)}\frac{d}{dr}\left(r\frac{dR}{dr}\right) + \frac{2M[E-V(r)]}{\hbar^2} r^2 &= F \quad (3) \end{aligned}\right\}$$

(2): $\frac{d^2P}{d\phi^2} = -FP$

$\Rightarrow P(\phi) = C_1 e^{im\phi}$ for $m = 0, \pm 1, \pm 2 ..$

(3): $\frac{1}{R(r)}\frac{d}{dr}\left(r\frac{dR}{dr}\right) + \frac{2M[E-V(r)]}{\hbar^2} r^2 = m^2$

$$\Rightarrow \begin{cases} r^2\frac{d^2R}{dr^2} + r\frac{dR}{dr} + \left[\frac{2M(E+V_0)}{\hbar^2} r^2 - m^2\right] R = 0 & (0 \leq r \leq a) \\ r^2\frac{d^2R}{dr^2} + r\frac{dR}{dr} + \left(\frac{2mE}{\hbar^2} r^2 - m^2\right) R = 0 & (r > a) \end{cases}$$

For $K = \frac{\sqrt{-2ME}}{\hbar}$ & $l = \frac{\sqrt{2M(E+V_0)}}{\hbar} \Rightarrow \begin{cases} r^2\frac{d^2R}{dr^2} + r\frac{dR}{dr} + (l^2r^2 - m^2)R = 0 & (0 \leq r \leq a) \\ r^2\frac{d^2R}{dr^2} + r\frac{dR}{dr} + (-K^2r^2 - m^2)R = 0 & (r > a) \end{cases}$

According to Bassel functions:

$$R(r) = \begin{cases} C_2 J_m(lr) + C_3 Y_m(lr) & (0 \leq r \leq a), \ r \to 0 \Rightarrow C_3 = 0 \\ C_4 I_m(Kr) + C_5 K_m(Kr) & (r > a), \ r \to \infty \Rightarrow C_4 = 0 \end{cases}$$

$$\Rightarrow R(r) = \begin{cases} C_2 J_m(lr) & (0 \leq r \leq a) \\ C_5 K_m(Kr) & (r > a) \end{cases}$$

The wave function are expected to be similar from both sides of $r = a$

$$\Rightarrow \begin{cases} \lim_{r \to a^-} \Psi(r,\phi,t) = \lim_{r \to a^+} \Psi(r,\phi,t) \\ \lim_{r \to a^-} \frac{\partial \Psi}{\partial r} = \lim_{r \to a^+} \frac{\partial \Psi}{\partial r} \end{cases}$$

$$\Leftrightarrow \begin{cases} \lim_{r \to a^-} R(r)P(\phi)T(t) = \lim_{r \to a^+} R(r)P(\phi)T(t) \\ \lim_{r \to a^-} R'(r)P(\phi)T(t) = \lim_{r \to a^+} R'(r)P(\phi)T(t) \end{cases} \Leftrightarrow \begin{cases} R(a^-) = R(a^+) \\ R'(a^-) = R'(a^+) \end{cases}$$

$\Rightarrow$ Boundary cons: $\begin{cases} C_2 J_m(la) = C_5 K_m(Ka) \\ C_2 l J'_m(la) = C_5 K K'_m(Ka) \end{cases} \Rightarrow \dfrac{l J'_m(la)}{J_m(la)} = \dfrac{K K'_m(Ka)}{K_m(Ka)}$

$\Rightarrow \dfrac{la J'_m(la)}{J_m(la)} = \dfrac{Ka K'_m(Ka)}{K_m(Ka)}$. For $z = la$ & $z_0 = \dfrac{a}{\hbar}\sqrt{2\mu V_0} \Rightarrow Ka = \sqrt{z_0^2 - z^2}$

$m=0$ for ground state $\Rightarrow \dfrac{z J'_0(z)}{J_0(z)} = \dfrac{\sqrt{z_0^2-z^2}\,K'_0(\sqrt{z_0^2-z^2})}{K_0(\sqrt{z_0^2-z^2})}$

$\Rightarrow$ There is always at least 1 bound state

4.52. a) $\Psi_{nlm}(r,\theta,\phi,t) = R_{nl}(r) Y_l^m(\theta,\phi) e^{-iE_nt/\hbar}$ (only take time indep. part).

$\Rightarrow \Psi_{321}(r,\theta,\phi) = R_{32}(r) Y_2^1(\theta,\phi)$

$$= \left[\frac{4}{81\sqrt{30a_0^3}}\left(\frac{r}{a_0}\right)^2 e^{-r/3a_0}\right]\left(-\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{i\phi}\right)$$

$$= \frac{-4}{81\sqrt{16\pi a_0^3}}\frac{r^2}{a_0^2} e^{-r/3a_0}\sin\theta\cos\theta e^{i\phi}$$

$$= \frac{-r^2}{81\sqrt{\pi a_0^7}} e^{-r/3a_0}\sin\theta\cos\theta e^{i\phi}$$

b) $\iiint |\Psi_{321}|^2 dV = \int_0^\pi\int_0^{2\pi}\int_0^\infty \left|\dfrac{-r^2}{81\sqrt{\pi a_0^7}} e^{-r/3a_0}\sin\theta\cos\theta e^{i\phi} e^{-iE_3t/\hbar}\right|^2 (r^2\sin\theta\, dr\, d\phi\, d\theta)$

$$= \int_0^\pi\int_0^{2\pi}\int_0^\infty \frac{r^4}{81^2\pi a_0^7} e^{-2r/3a_0}\sin^2\theta\cos^2\theta(r^2\sin\theta\, dr\, d\phi\, d\theta)$$

$u = \cos^2\theta$, $v = \dfrac{2}{3a_0} \Rightarrow \iiint|\Psi_{321}|^2 dV = \dfrac{2}{6561a_0^7}\cdot\dfrac{4}{15}\cdot\dfrac{720}{2^7}3^7a_0^7$ (after integrating by parts) $= 1$.

$\Rightarrow \Psi_{321}$ is normallized.

c) $\langle r^s\rangle = \dfrac{\langle\Psi_{321}|r^s|\Psi_{321}\rangle}{\langle\Psi_{321}|\Psi_{321}\rangle} = \dfrac{\iiint \Psi_{321}^* r^s \Psi_{321}\, dV}{\iiint \Psi_{321}^*\Psi_{321}\, dV} = \int_0^\pi\int_0^{2\pi}\int_0^\infty r^s|\Psi_{321}(r,\theta,\phi)e^{-iE_3t/\hbar}|^2(r^2\sin\theta\, dr\, d\phi\, d\theta)$

$$= \int_0^\pi\int_0^{2\pi}\int_0^\infty r^s\left|\frac{-r^2}{81\sqrt{\pi a_0^7}} e^{-r/3a_0}\sin\theta\cos\theta\, 1\, e^{i\phi} e^{-iE_3t/\hbar}\right|^2(r^2\sin\theta\, dr\, d\phi\, d\theta)$$

$= \dfrac{8}{98415a_0^7}\displaystyle\int_0^\infty r^{s+6}e^{-2r/3a_0}dr$, $v = \dfrac{2r}{3a_0}$, $r = \dfrac{3a_0v}{2}$

$\Rightarrow \langle r^s\rangle = \dfrac{8}{98415a_0^7}\displaystyle\int_0^\infty\left(\frac{3a_0v}{2}\right)^{s+6}e^{-v}\left(\frac{3a_0}{2}dv\right) = \frac{1}{720}\left(\frac{3a_0}{2}\right)^s\Gamma(s+7)$

$\Rightarrow s > -7$ to satisfied the gamma function (also the range of s for $\langle r^s\rangle$)

4.71. $\psi_{2px}(r,\theta,\phi) = \frac{1}{\sqrt{32\pi a^3}} \frac{x}{a} e^{-r/2a}$, same with y, z but with $\frac{y}{a}, \frac{z}{a}$

a) $\psi_{2px} = \frac{1}{\sqrt{32\pi a^3}} \frac{x}{a} e^{-r/2a} = C_1 \psi_{21-1} + C_2 \psi_{210} + C_3 \psi_{211}$

$= C_1 R_{21} Y_1^{-1} + C_2 R_{21} Y_1^0 + C_3 R_{21} Y_1^1$

$= C_{21} (C_1 Y_1^{-1} + C_2 Y_1^0 + C_3 Y_1^1)$

$= \frac{1}{2\sqrt{6}} a^{-3/2} \left(\frac{r}{a}\right) e^{-r/2a} \left[C_1 \sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\phi} + C_2 \sqrt{\frac{3}{4\pi}} \cos\theta - C_3 \sqrt{\frac{3}{8\pi}} \sin\theta e^{i\phi} \right]$

$= \frac{1}{\sqrt{32\pi a^3}} \frac{r}{a} e^{-r/2a} \left(\frac{C_1}{\sqrt{2}} \sin\theta e^{-i\phi} + C_2 \cos\theta - \frac{C_3}{\sqrt{2}} \sin\theta e^{i\phi} \right)$

$C_1 = 1/\sqrt{2}, C_2 = 0, C_3 = -1/\sqrt{2} \Rightarrow \psi_{2px} = \frac{1}{\sqrt{32\pi a^3}} \frac{r}{a} e^{-r/2a} \left(\frac{1}{2} \sin\theta e^{-i\phi} + \frac{1}{2} \sin\theta e^{i\phi} \right)$

$\Rightarrow \psi_{2px} = \frac{1}{\sqrt{32\pi a^3}} \frac{r\sin\theta}{a} e^{-r/2a} \cos\phi = \frac{1}{\sqrt{32\pi a^3}} \frac{x}{a} e^{-r/2a}$

$= \left(\frac{1}{\sqrt{2}}\right) \psi_{21-1} + 0 \cdot \psi_{210} + \left(\frac{-1}{\sqrt{2}}\right) \psi_{211}$

* Similar with ψ_{2py} but $C_1 = -1/\sqrt{2}i$, $C_2 = 0$, $C_3 = -1/\sqrt{2}i$

$\Rightarrow \psi_{2py} = \frac{-1}{i\sqrt{2}} \psi_{21-1} + 0 \cdot \psi_{210} + \frac{-1}{i\sqrt{2}} \psi_{211}$

* Similar with ψ_{2pz} but $C_1 = 0$, $C_2 = 1$, $C_3 = 0$

$\Rightarrow \psi_{2pz} = 0 \cdot \psi_{21-1} + 1 \cdot \psi_{210} + 0 \cdot \psi_{211}$

b) $L_x \psi_{2px} = -i\hbar \left(-\sin\phi \frac{\partial}{\partial\theta} - \cos\phi \cot\theta \frac{\partial}{\partial\phi} \right) \psi_{2px}$

$= i\hbar \left(\sin\phi \frac{\partial}{\partial\theta} + \cos\phi \cot\theta \frac{\partial}{\partial\phi} \right) \left(\frac{1}{\sqrt{2}} \psi_{21-1} - \frac{1}{\sqrt{2}} \psi_{211} \right)$

$= \frac{i\hbar}{\sqrt{2}} \left(\sin\phi \frac{\partial}{\partial\theta} + \cos\phi \cot\theta \frac{\partial}{\partial\theta} \right) \left[R_{21}(r) Y_1^{-1}(\theta,\phi) - R_{21}(r) Y_1^{1}(\theta,\phi) \right]$

$= i\hbar R_{21}(r) \sqrt{\frac{3}{16\pi}} \left(\sin\phi \frac{\partial}{\partial\theta} + \cos\phi \cot\theta \frac{\partial}{\partial\phi} \right) \sin\theta (e^{-i\phi} + e^{i\phi})$

$= i\hbar R_{21}(r) \sqrt{\frac{3}{16\pi}} \left(\sin\phi \frac{\partial}{\partial\theta} + \cos\phi \cot\theta \frac{\partial}{\partial\phi} \right) \sin\theta \, 2\cos\phi$

$= i\hbar R_{21}(r) \sqrt{\frac{3}{4\pi}} \left[\sin\phi (\cos\phi \cos\theta) + \cos\phi \cot\theta (-\sin\theta \sin\phi) \right]$

$= i\hbar R_{21}(r) \sqrt{\frac{3}{4\pi}} (\sin\phi \cos\theta \cos\phi - \sin\phi \cos\theta \cos\phi) = 0 = 0 \cdot \psi_{2px}$

$\Rightarrow$ ψ_{2px} is an eigenfunction of L_x with eigenvalue 0.

Similarly:

ψ_{2py} is an eigenfunction of L_y with eigenvalue 0

ψ_{2pz} is an eigenfunction of L_z with eigenvalue 0

c) (Mercy, I don't want to graph).

4.73. $H = \frac{p^2}{2m} - \gamma \vec{B}\cdot\vec{S}$, $m \frac{d^2}{dt^2}\langle z\rangle = \gamma\alpha\langle S_z\rangle$

$$\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle + \left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle$$

$$\Leftrightarrow \frac{d}{dt}\langle z\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{z}]\rangle + \underbrace{\left\langle\frac{\partial z}{\partial t}\right\rangle}_{=0} = \frac{i}{\hbar}\left\langle\left[\frac{p^2}{2m} - \gamma\vec{B}\cdot\vec{S}, z\right]\right\rangle = \frac{i}{\hbar}\left\langle\left[\frac{p^2}{2m}, z\right] - [\gamma\vec{B}\cdot\vec{S}, z\right.$$

$$= \frac{i}{2m\hbar}\langle\underbrace{[p^2,z]}_{=[p_x^2+p_y^2+p_z^2,\, z]}\rangle - \frac{i\gamma}{\hbar}\langle[\vec{B}\cdot\vec{S}, z]\rangle$$

$$= \frac{i}{2m\hbar}\langle p_x\underbrace{[p_x,z]}_{0} + \underbrace{[p_x,z]}_{0}p_x + p_y\underbrace{[p_y,z]}_{0} + \underbrace{[p_y,z]}_{0}p_y + p_z\underbrace{[p_z,z]}_{-i\hbar} + \underbrace{[p_z,z]}_{-i\hbar}p_z\rangle - \frac{i\gamma}{\hbar}\langle[\vec{B}\cdot\vec{S}, z]\rangle$$

$$= \frac{i}{2m\hbar}\langle -2i\hbar p_z\rangle - \frac{i\gamma}{\hbar}\langle[\vec{B}\cdot\vec{S}, z]\rangle = \frac{1}{m}\langle p_z\rangle - \frac{i\gamma}{\hbar}\langle\psi|[\vec{B}\cdot\vec{S}, z]|\psi\rangle$$

$$= \frac{1}{m}\langle p_z\rangle - \frac{i\gamma}{\hbar}\iiint \underbrace{\psi^\dagger[\vec{B}\cdot\vec{S}, z]\psi\, dV}_{= \begin{bmatrix}\psi_+\\ \psi_-\end{bmatrix}^\dagger[(\vec{B}\cdot\vec{S})z - z(\vec{B}\cdot\vec{S})]\begin{bmatrix}\psi_+\\ \psi_-\end{bmatrix}dV}$$

$$= \frac{1}{m}\langle p_z\rangle - \frac{i\gamma}{\hbar}\iiint\begin{bmatrix}\psi_+\\ \psi_-\end{bmatrix}^\dagger\left\{\frac{\hbar}{2}\begin{bmatrix}B_0+\alpha z & -\alpha x\\ -\alpha x & -B_0-\alpha z\end{bmatrix}z - z\frac{\hbar}{2}\begin{bmatrix}B_0+\alpha z & -\alpha x\\ -\alpha x & -B_0-\alpha z\end{bmatrix}\right\}\begin{bmatrix}\psi_+\\ \psi_-\end{bmatrix}dV$$

$$= \frac{1}{m}\langle p_z\rangle - \frac{i\gamma}{2}\iiint\begin{bmatrix}\psi_+\\ \psi_-\end{bmatrix}^\dagger\begin{bmatrix}0 & 0\\ 0 & 0\end{bmatrix}\begin{bmatrix}\psi_+\\ \psi_-\end{bmatrix}dV = \frac{1}{m}\langle p_z\rangle$$

$$\Rightarrow m\frac{d}{dt}\langle z\rangle = \langle p_z\rangle \Leftrightarrow \frac{d}{dt}\left(m\frac{d}{dt}\langle z\rangle\right) = \frac{d}{dt}\langle p_z\rangle \Leftrightarrow m\frac{d^2}{dt^2}\langle z\rangle = \frac{i}{\hbar}\langle[\hat{H}, p_z]\rangle + \underbrace{\left\langle\frac{\partial p_z}{\partial t}\right\rangle}_{=0}$$

$$= \frac{i}{\hbar}\left\langle\left[\frac{p^2}{2m}, p_z\right] - [\gamma\vec{B}\cdot\vec{S}, p_z]\right\rangle = \frac{i}{\hbar}\left\langle\frac{1}{2m}\underbrace{[p^2, p_z]}_{=[p_x^2+p_y^2+p_z^2,\, p_z]} - \gamma[\vec{B}\cdot\vec{S}, p_z]\right\rangle$$

$$\Rightarrow m\frac{d^2}{dt^2}\langle z\rangle = \frac{i}{\hbar}\left\langle\frac{1}{2m}(\underbrace{[p_x^2, p_x]}_{=0} + \underbrace{[p_y^2, p_y]}_{=0} + \underbrace{[p_z^2, p_z]}_{=0}) - \gamma\underbrace{[\vec{B}\cdot\vec{S}, p_z]}_{=\psi^\dagger[(\vec{B}\cdot\vec{S})p_z - p_z(\vec{B}\cdot\vec{S})]\psi}\right\rangle$$

$$= \frac{-i\gamma}{\hbar}\langle[\vec{B}\cdot\vec{S}, p_z]\rangle = \frac{-i\gamma}{\hbar}\langle\psi|\vec{B}\cdot\vec{S}, p_z]|\psi\rangle$$

$$= \frac{-i\gamma}{2}\iiint\begin{bmatrix}\psi_+\\ \psi_-\end{bmatrix}^\dagger\left\{\begin{bmatrix}B_0+\alpha z & -\alpha x\\ -\alpha x & -B_0-\alpha z\end{bmatrix}\left(-i\hbar\frac{\partial}{\partial z}\right) - \left(-i\hbar\frac{\partial}{\partial z}\right)\begin{bmatrix}B_0+\alpha z & -\alpha x\\ -\alpha x & -B_0-\alpha z\end{bmatrix}\right\}\begin{bmatrix}\psi_+\\ \psi_-\end{bmatrix}dV$$

$$= \frac{\hbar\gamma}{2}\iiint\begin{bmatrix}\psi_+\\ \psi_-\end{bmatrix}^\dagger\left\{\begin{bmatrix}(-B_0-\alpha z)\frac{\partial\psi_+}{\partial z} + \alpha x\frac{\partial\psi_-}{\partial z}\\ \alpha x\frac{\partial\psi_+}{\partial z} + (B_0+\alpha z)\frac{\partial\psi_-}{\partial z}\end{bmatrix} + \begin{bmatrix}(B_0+\alpha z)\frac{\partial\psi_+}{\partial z} + \alpha\psi_+ - \alpha x\frac{\partial\psi_-}{\partial z}\\ -\alpha x\frac{\partial\psi_+}{\partial z} + (-B_0-\alpha z)\frac{\partial\psi_-}{\partial z} - \alpha\psi_-\end{bmatrix}\right\}dV$$

$$= \frac{\hbar\gamma}{2}\iiint\begin{bmatrix}\psi_+\\ \psi_-\end{bmatrix}^\dagger\begin{bmatrix}\alpha\psi_+\\ -\alpha\psi_-\end{bmatrix}dV = \frac{\hbar\gamma\alpha}{2}\iiint\begin{bmatrix}\psi_+\\ \psi_-\end{bmatrix}^\dagger\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\begin{bmatrix}\psi_+\\ \psi_-\end{bmatrix}dV$$

$$= \gamma\alpha\iiint\psi^\dagger S_z\psi\, dV = \gamma\alpha\langle\psi|S_z|\psi\rangle = \gamma\alpha\langle S_z\rangle$$