سؤال اول

$$V(r) = \begin{cases} -V_0 & r<a \\ 0 & r>a \end{cases}$$

انرژی مقید $-V_0 \leq E \leq 0$

$$-\frac{\hbar^2}{2m}\left[\frac{d^2R_{nl}(r)}{dr^2} + \frac{2}{r}\frac{dR_{nl}(r)}{dr} - \frac{l(l+1)}{r^2}R_{nl}(r)\right] - (E - V(r))R_{nl}(r) = 0$$

$$\frac{2mE}{\hbar^2} = -q^2 \quad , \quad \frac{2m(E+V_0)}{\hbar^2} = k^2$$

$(r<a)$
$$\frac{d^2R_{nl}}{dr^2} + \frac{2}{r}\frac{dR_{nl}}{dr} - \frac{2}{r^2}R_{nl} + k^2R_{nl} = 0$$

$$R_{nl}(r) = A\,j_1(kr) + \cancel{B\,n_1(kr)}$$

$\xrightarrow{} 0$ در $r=0$ نامتناهی می‌شود.

$(r>a)$
$$\frac{d^2R_{nl}}{dr^2} + \frac{2}{r}\frac{dR_{nl}}{dr} - \frac{2}{r^2}R_{nl} - q^2R_{nl} = 0$$

$$R_{nl}(r) = C\,h_1^{(1)}(iqr) + \cancel{D\,h_1^{(2)}(iqr)}$$

$\xrightarrow{} 0$ در $r \to +\infty$ نامتناهی می‌شود.

شرط مرزی در $r=a$:

$$\frac{1}{j_1(kr)}\frac{dj_1(kr)}{dr}\bigg|_{r=a} = \frac{1}{h_1^{(1)}(iqr)}\frac{dh_1^{(1)}(iqr)}{dr}\bigg|_{r=a}$$

می‌توان به صورت زیر نوشت:

$$\frac{k}{j_1(\rho)}\frac{dj_1(\rho)}{d\rho}\bigg|_{\rho=ka} = \frac{iq}{h_1^{(1)}(\rho)}\frac{dh_1^{(1)}(\rho)}{d\rho}\bigg|_{\rho=iqa}$$

$$j_1(\rho) = \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho} \quad , \quad \frac{dj_1(\rho)}{d\rho} = \frac{2\cos\rho}{\rho^2} - \frac{2\sin\rho}{\rho^3} + \frac{\sin\rho}{\rho}$$

$$h_1^{(1)}(\rho) = -\frac{e^{i\rho}}{\rho}\left(1+\frac{i}{\rho}\right) \quad , \quad \frac{dh_1^{(1)}(\rho)}{d\rho} = e^{i\rho}\left(-\frac{i}{\rho} + \frac{2}{\rho^2} + \frac{2i}{\rho^3}\right)$$

$$k \, \frac{\dfrac{2\cos\rho}{\rho^2} - \dfrac{2\sin\rho}{\rho^3} + \dfrac{\sin\rho}{\rho}}{\dfrac{\sin\rho}{\rho^2} - \dfrac{\cos\rho}{\rho}}\Bigg|_{\rho=ka} = iq \, \frac{e^{i\rho}\left(-\frac{i}{\rho}+\frac{2}{\rho^2}+\frac{2i}{\rho^3}\right)}{-e^{i\rho}\left(\frac{1}{\rho}+\frac{i}{\rho^2}\right)}\Bigg|_{\rho=iqa}$$

$$\frac{k}{\rho} \, \frac{2\rho+(\rho^2-2)\tan\rho}{\tan\rho-\rho}\Bigg|_{\rho=ka} = \frac{iq}{\rho}\left(\frac{i\rho^2-2\rho-2i}{\rho+i}\right)\Bigg|_{\rho=iqa}$$

به ازای انرژی بستگی صفر یعنی E=0 داریم:

$$q_0=0 \quad , \quad K_0^2 = \frac{2mV_0}{\hbar^2}$$

$$\frac{k_0}{k_0a} \, \frac{2k_0a+[(k_0a)^2-2]\tan k_0a}{\tan k_0a - k_0a} = -\frac{2}{a}$$

$$\cancel{2k_0a} + ((k_0a)^2 \cancel{-2})\tan k_0a = \cancel{-2\tan k_0a} + \cancel{2k_0a}$$

$$(k_0a)^2 \tan k_0a = 0 \quad \rightarrow \quad \tan k_0a = 0$$

از حل این معادله V_0 ها بدست می آید.

Q(3)

$a < r < b$: $\frac{d^2 U_{n0}(r)}{dr^2} + k^2 U_{n0}(r) = 0$

$$\left.\begin{array}{l} U_{n0}(r) = r R_{n0}(r) \\ k^2 = \frac{2mE}{\hbar^2} \end{array}\right\} \Rightarrow U_{n0}(r) = A\sin[k(r-a)]$$

حال با استفاده از شرایط مرزی :

$$U_{n0}(r)\Big|_{r=b} = 0 \Rightarrow A\sin[k(b-a)] = 0 \Rightarrow k(b-a) = n\pi$$

$$\Rightarrow E_n = \frac{\hbar^2 k^2}{2m} = \boxed{\frac{n^2\pi^2\hbar^2}{2m(a-b)^2} = E_n}$$

از طرفی :
$$1 = \int_a^b r^2 R_{n0}(r)dr = \int_a^b A^2 \sin^2[k(r-a)]dr$$

$$= \frac{A^2}{2}\int_a^b \{1 - \cos[2k(r-a)]dr = \boxed{\frac{b-a}{2}A^2 = 1}$$

$$\boxed{\Rightarrow R_{n0} = \frac{U_{n0}(r)}{r} = \begin{cases} \sqrt{\frac{2}{b-a}}\,\frac{1}{r}\sin\left[\frac{n\pi(r-a)}{b-a}\right] & r<a<b \\ 0, & \text{elsewhere} \end{cases}}$$

$$\Rightarrow \Psi_{n00} = \frac{1}{\sqrt{4\pi}} R_{n0}(r)$$

Q(4):

i) $n=1\,,\ \ell=0\ :\quad R_{10}(r)=2a_0^{-3/2}\,e^{-r/a_0}$

$$\Rightarrow P_{10}=r^2|R_{10}|^2=\frac{4}{a_0^3}\,r^2e^{-2r/a_0}$$

$$\left.\frac{dP_{10}(r)}{dr}\right|_{r=r_1}=0\Rightarrow 2r_1-\frac{2r_1^2}{a_0}=0\Rightarrow\boxed{r_1=a_0}$$

ii) $$R_{21}(r)=\frac{1}{2\sqrt{6}\,a_0^{5/2}}\,r\,e^{-\frac{r}{2a_0}}$$

$$P_{12}(r)=r^2|R_{21}|^2=\frac{1}{24a_0^5}\,r^4e^{-\frac{r}{a_0}}$$

$$\left.\frac{dP_{12}(r)}{dr}\right|_{r=r_2}=0\Rightarrow 4r_2^3-\frac{r_2^4}{a_0}=0\Rightarrow\boxed{r_2=4a_0}$$

iii) $$R_{n(n-1)}(r)=-\left(\frac{2}{na_0}\right)^{3/2}\frac{1}{\sqrt{2n[(2n-1)!]^3}}\left(\frac{2r}{na_0}\right)^{n-1}e^{-\frac{r}{na_0}}L_{2n-1}^{2n-1}\left(\frac{2r}{na_0}\right)$$

اگر همه‌ی ثابت‌ها را با A_n نشان دهیم، داریم:

$$P_{n(n-1)}(r)=r^2|R_{n(n-1)}(r)|^2=A_n^2\,r^{2n}e^{-2r/na_0}$$

$$\left.\frac{dP_{n(n-1)}(r)}{dr}\right|_{r=r_n}=0\Rightarrow 2n\,r_n^{2n-1}-\frac{2r_n^{2n}}{na_0}=0\Rightarrow\boxed{r_n=n^2a_0}$$

سؤال 5 : حالات ویژه انرژی را می‌توان به صورت زیر نوشت :

$$|\psi_E\rangle = |n_x\rangle \otimes |n_y\rangle \otimes |n_z\rangle$$

$$\Rightarrow E = \hbar\omega_x(n_x + 1/2) + \hbar\omega_y(n_y + 1/2) + \hbar\omega_z(n_z + 1/2)$$

ب)

$$[L_z, P^2] = [L_z, z^2] = 0 \,,\; [L_z, r^2] = 0 \Rightarrow [L_z, x^2 + y^2] = 0$$

$$\Rightarrow [H, L_z] = \left[\frac{P^2}{2m} + \frac{1}{2}m(\omega_x^2 X^2 + \omega_y^2 Y^2 + \omega_z^2 Z^2)\right] = \begin{cases} 0 & \text{اگر } \omega_x = \omega_y \\ \text{غیر صفر} & \text{اگر } \omega_x \neq \omega_y \end{cases}$$

$$\Rightarrow [L^2, X^2] = [L^2, Z^2] = [L^2, Y^2] \neq 0$$

$$[L^2, P^2] = 0 \,,\; [L^2, R^2] = 0 \Rightarrow \begin{cases} [H, L^2] = 0 & \text{اگر } \omega_x = \omega_y = \omega_z \\ [H, L^2] \neq 0 & \text{اگر هر سه } \omega \text{ ها یکی نباشند} \end{cases}$$

اگر هر سه ω ها یکی باشند H هم با L_z و هم با L^2 ویژه بردار مشترک دارد . اگر فقط $\omega_x = \omega_y$ ، H با L_z ویژه بردار مشترک دارد .

ج)

$$E = \hbar\omega\left(n_x + n_y + \tfrac{3}{2}n_z + \tfrac{7}{4}\right) \,,\; n = n_x + n_y + \tfrac{3}{2}n_z$$

$E_0 = E_{000} = \frac{7}{4}\hbar\omega$ تبهگنی ندارد

$E_1 = E_{100} = E_{010} = \frac{11}{4}\hbar\omega$ تبهگنی دوگانه

$E_2 = E_{001} = \frac{13}{4}\hbar\omega$ تبهگنی ندارد .

سؤال 6:

الف)
$$\int |\psi|^2 dv = 1 \rightarrow |N|^2 \int r^2 e^{-r/a_0} r^2 dr \int |Y_{1,-1}|^2 d\Omega = |N|^2 \int r^4 e^{-r/a_0} dr = 24 a_0^5 |N|^2$$

$$\rightarrow \int_0^\infty r^4 e^{-\alpha r} dr = \frac{\partial^4}{\partial \alpha^4} \int_0^\infty e^{-\alpha r} dr = \frac{\partial^4}{\partial \alpha^4} \frac{1}{\alpha}$$

$$|N| = \frac{1}{2a_0^2\sqrt{6a_0}}$$

ب) $r = a_0$: جایی که $|\psi|^2$ ماکزیمم است

$$p = N^2 r^2 e^{-r/a_0} |Y_{1,-1}|^2 = \frac{1}{24 a_0^5} a_0^2 e^{-1} \left(\sqrt{\frac{3}{8\pi}} \sin 45\right)^2 = \frac{1}{128\pi e a_0^3}$$

$$p = r^2 |R_{21}|^2 = N^2 r^4 e^{-r/a_0} = \frac{2}{3 a_0 e^2}$$

ج)
$$Y_{lm} = Y_{1,-1} \rightarrow l=1, m=-1 \rightarrow L_z \in \left\{ \frac{-\hbar}{2} \right\} , \quad L^2 = 1(1+1)\hbar^2 = 2\hbar^2$$

سؤال هفتم :

$\psi_{n,l,m} \longrightarrow |n,l,m\rangle$

$$|\psi(0)\rangle = \frac{1}{\sqrt{10}}\left(2|1,0,0\rangle + |2,1,0\rangle + \sqrt{2}\,|2,1,1\rangle + \sqrt{3}\,|2,1,-1\rangle\right)$$

الف/ $H|n,l,m\rangle = E_n|n,l,m\rangle \qquad E_n = \frac{-E_I}{n^2}$

$$\langle E\rangle = \langle\psi|H|\psi\rangle = \frac{4}{10}E_1 + \left(\frac{1}{10}+\frac{2}{10}+\frac{3}{10}\right)E_2$$

$$= \frac{1}{5}(2E_1 + 3E_2) = \frac{1}{5}\left(2(-E_I) + 3\left(-\frac{E_I}{4}\right)\right) = -E_I\left(\frac{2}{5}+\frac{3}{20}\right)$$

$$= -0.55\,E_I = -0.55\,(13.6\ eV) = -7.47\ eV$$

ب/ $P(l=1,m=1) = |\langle n,1,1|\psi(t)\rangle|^2$

$$|\psi(t)\rangle = e^{-itH/\hbar}|\psi(0)\rangle = \frac{1}{\sqrt{10}}\left(2e^{-itE_1/\hbar}|1,0,0\rangle + \sqrt{2}e^{-itE_2/\hbar}|2,1,0\rangle\right.$$

$$\left. + \sqrt{2}e^{-iE_2t/\hbar}\,\underline{|2,1,1\rangle} + \sqrt{3}e^{-iE_2t/\hbar}|2,1,-1\rangle\right)$$

$$\longrightarrow P(l,m=1) = \left|\frac{\sqrt{2}}{\sqrt{10}}e^{-iE_2t/\hbar}\right|^2 = \frac{2}{10} = \frac{1}{5}$$

ج/ L^2 ویژه مقدار : $\hbar^2 l(l+1) \longrightarrow \sqrt{2}\hbar = \hbar\sqrt{l(l+1)} \longrightarrow l=1$

$\longrightarrow n \geq 2$

با توجه به مقادیر n در $|\psi\rangle$ $\longrightarrow \underline{n=2}$

$L_x|\psi\rangle = +\hbar|\psi\rangle$

پس از اندازه گیری حالت سیستم ترکیب خطی $|2,1,0\rangle$ ، $|2,1,1\rangle$ و $|2,1,-1\rangle$ است :

$$\boxed{|\psi\rangle = \alpha|2,1,0\rangle + \beta|2,1,1\rangle + \gamma|2,1,-1\rangle}$$

$$L_x|\psi\rangle = \hbar\left(\frac{\sqrt{2}}{2}\alpha|2,1,1\rangle + \frac{\sqrt{2}}{2}(\beta+\gamma)|2,1,0\rangle + \frac{\sqrt{2}}{2}\alpha|2,1,-1\rangle\right) = \hbar|\psi\rangle$$

$\longrightarrow \alpha = \frac{\sqrt{2}}{2}(\beta+\gamma)$

$\beta = \frac{\sqrt{2}}{2}\alpha = \gamma \quad , \quad \alpha^2+\beta^2+\gamma^2 = 1 \longrightarrow \boxed{\alpha = \frac{1}{\sqrt{2}} \quad \beta = \gamma = \frac{1}{2}}$