- Атом водоника -

$$\hat{H}\Psi = E\Psi \qquad E = -\frac{1}{(4\pi\varepsilon_0)^2}\frac{\mu Z^2 e^4}{2\hbar^2 n^2}$$

$$n = 1, 2, 3 \ldots$$

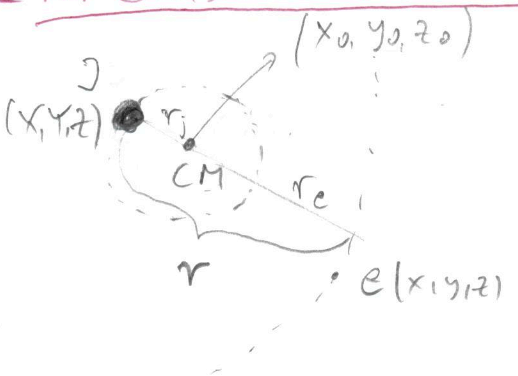
$$r_n = 4\pi\varepsilon_0 \frac{n^2\hbar^2}{Ze^2\mu} = a_0 n^2$$

$$\hat{H} = \hat{T}_J + \hat{T}_e + \hat{U}$$

$$\Big[-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial X^2}+\frac{\partial^2}{\partial Y^2}+\frac{\partial^2}{\partial Z^2}\right) - \frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) -$$

$$- \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{\sqrt{(x-X)^2+(y-Y)^2+(z-Z)^2}}\Big]\Psi = E\Psi$$

- Прелазак у систем центра масе



$$MX + mx = (M+m)x_0$$

$$MY + my = (M+m)y_0$$

$$MZ + mz = (M+m)z_0$$

$$x_0 = \frac{M}{m+M}X + \frac{m}{m+M}x \qquad x - X = x_r$$

$$y_0 = \frac{M}{m+M}Y + \frac{m}{m+M}y \qquad y - Y = y_r$$

$$z_0 = \frac{M}{m+M}Z + \frac{m}{m+M}z \qquad z - Z = z_r$$

$$\frac{\partial}{\partial X} = \frac{\partial x_0}{\partial X}\frac{\partial}{\partial x_0} + \frac{\partial x_r}{\partial X}\frac{\partial}{\partial x_r} = \frac{M}{M+m}\frac{\partial}{\partial x_0} - \frac{\partial}{\partial x_r}$$

$$\frac{\partial^2}{\partial X^2} = \frac{\partial}{\partial X}\frac{\partial}{\partial X} = \left(\frac{\partial x_0}{\partial X}\frac{\partial}{\partial x_0} + \frac{\partial x_r}{\partial X}\frac{\partial}{\partial x_r}\right)\left(\frac{M}{M+m}\frac{\partial}{\partial x_0} - \frac{\partial}{\partial x_r}\right) =$$

$$= \left(\frac{M}{M+m}\right)^2\frac{\partial^2}{\partial x_0^2} - \frac{2M}{M+m}\frac{\partial}{\partial x_0}\frac{\partial}{\partial x_r} + \frac{\partial^2}{\partial x_r^2}$$

$$\frac{\partial x_0}{\partial X} = \frac{M}{M+m} \qquad \frac{\partial x_r}{\partial X} = -1$$

$$\frac{\partial^2}{\partial x^2} = \left(\frac{m}{M+m}\right)^2\frac{\partial^2}{\partial x_0^2} + \frac{2m}{M+m}\frac{\partial}{\partial x_0}\frac{\partial}{\partial x_r} + \frac{\partial^2}{\partial x_r^2}$$

$$-\frac{\hbar^2}{2(M+m)}\left(\frac{\partial^2}{\partial x_0^2}+\frac{\partial^2}{\partial y_0^2}+\frac{\partial^2}{\partial z_0^2}\right)\Psi - \frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x_r^2}+\frac{\partial^2}{\partial y_r^2}+\frac{\partial^2}{\partial z_r^2}\right)\Psi$$

$$-\frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{\sqrt{x_r^2+y_r^2+z_r^2}}\Psi = E\Psi \qquad \mu = \frac{mM}{M+m}$$

$$\Psi(x_0,y_0,z_0,x_r,y_r,z_r) = \Psi_1(x_0,y_0,z_0)\,\Psi_2(x_r,y_r,z_r)$$

1) $$-\frac{\hbar^2}{2(M+m)}\left(\frac{\partial^2}{\partial x_0^2}+\frac{\partial^2}{\partial y_0^2}+\frac{\partial^2}{\partial z_0^2}\right)\Psi_1 = E_1\Psi_1$$

$\downarrow$

$$\Psi_1 = \Psi_1'(x_0)\,\Psi_2'(y_0)\,\Psi_3'(z_0) \qquad E_1 = E_x' + E_y' + E_z'$$

$$\Psi_1'(x_0) = C_1 e^{+\frac{i}{\hbar}p_x x_0} + C_2 e^{-\frac{i}{\hbar}p_x x_0} \qquad p_x = \sqrt{2(M+m)\underbrace{E_x}_{\text{транслационог}}}$$

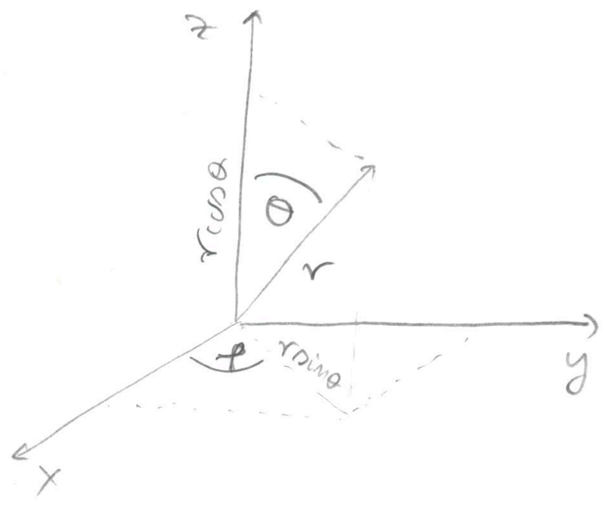
E_1 – допринос енергији атома H због слободног кретања атома.

↳ није квантована

↳ структура енергетских нивоа је одређена Кулоновим потенцијалом.

- прелазак у сферне координате

$$-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\Psi - \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r}\Psi = E\Psi$$



$$r = \sqrt{x^2+y^2+z^2}$$

$x = r\sin\theta\cos\varphi \qquad 0 < r < \infty$

$y = r\sin\theta\sin\varphi \qquad 0 \le \varphi < 2\pi$

$z = r\cos\theta \qquad 0 \le \theta \le \pi$

$$\theta = \operatorname{arctg}\frac{\sqrt{x^2+y^2}}{z}$$

$$\varphi = \operatorname{arctg}\frac{y}{x}$$

$$\left(-\frac{\hbar^2}{2\mu}\Delta - \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r}\right)\psi = E\psi \qquad \begin{cases} \frac{\partial r}{\partial x} = \sin\theta\cos\varphi \\ \frac{\partial \theta}{\partial x} = \frac{\cos\theta\cos\varphi}{r} \\ \frac{\partial \varphi}{\partial x} = -\frac{\sin\varphi}{r\cos\theta} \end{cases}$$

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial \theta}{\partial x}\frac{\partial}{\partial \theta} + \frac{\partial \varphi}{\partial x}\frac{\partial}{\partial \varphi} \qquad \frac{\partial^2}{\partial x^2} = \frac{\partial}{\partial x}\frac{\partial}{\partial x}$$

$\downarrow$

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]$$

$$\psi(r,\theta,\varphi) = R(r)S(\theta,\varphi)$$

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{dR}{dr}\right) + \frac{2\mu}{\hbar^2}\left(E + \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r}\right) = f$$

$$\frac{1}{\sin^2\theta}\frac{1}{S}\frac{\partial^2 S}{\partial\varphi^2} + \frac{1}{\sin\theta}\frac{1}{S}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial S}{\partial\theta}\right) = -f$$

$\downarrow$

$$S(\theta,\varphi) = \Phi(\varphi)\Theta(\theta)$$

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\varphi^2} + \frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + f\sin^2\theta = 0$$

$$\frac{d^2\Phi}{d\varphi^2} + m^2\Phi = 0$$

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \left(f - \frac{m^2}{\sin^2\theta}\right)\Theta = 0$$

$$\Phi(\varphi) = A e^{\alpha\varphi} = A e^{im\varphi}$$

$$e^{im\varphi} = e^{im(\varphi+2\pi)} . \quad 1 = \cos 2m\pi + i\sin 2m\pi$$

$$m = 0, \pm 1, \pm 2, \pm 3 \ldots$$

$$\Phi = \frac{1}{\sqrt{2\pi}} e^{im\varphi}$$

$$R_{n,l}(r) = \sqrt{\left(\frac{2Z}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}}\; e^{-\frac{Z}{na_0}r}\left(\frac{2Z}{na_0}r\right)^l L^{2l+1}_{n-l-1}\left(\frac{2Z}{na_0}r\right)$$

$$R_{n,l}(\rho) = \sqrt{\left(\frac{2Z}{na_0}\right)^3 \frac{n-l-1}{2n[(n+l)!]^3}}\; e^{-\rho}\rho^l L^{2l+1}_{n-l-1}(\rho)$$

$$\rho = \frac{2Z}{na_0}r$$

$$L_q(\rho) = e^{\rho}\left(\frac{d}{d\rho}\right)^q\left(e^{-\rho}\rho^q\right)$$

$$L^{p\;\,2l+1}_{\underbrace{n-l+1}_{q-p}}(\rho) = (-1)^p\left(\frac{d}{d\rho}\right)^p L_q(\rho)$$

$$\boxed{\begin{array}{l} L^{2l+1}_{n+l} \\ q = n+l \qquad p = 2l+1 \end{array}}$$