

II ROTATIONAL

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IN THE CASE OF ROTATIONS WE CONSIDER THE ELECTRIC FIELD IN THE \hat{z} -DIRECTION

$$\vec{E}(t) = |E_0| \hat{K} \cos(\omega t)$$

THEREFORE

$$\vec{\mu} \cdot \vec{E} \approx |E_0| \frac{\mu}{z} \cos(\omega t)$$

AND

$$\frac{\mu}{z} = \mu^0 + \left. \frac{d\mu}{dz} \right|_0 z + \frac{1}{2} \left. \frac{d^2\mu}{dz^2} \right|_0 z^2 + \dots$$

NOW

$$z = r \cos\theta \sim r y_1^0(\theta, \varphi)$$

$$\hat{h}_{10} \rightarrow \langle l', m' | \hat{h}(z) | l, m \rangle$$

$$\langle l', m' | |E_0| g \frac{\mu}{z} | l, m \rangle = g |E_0| \langle l', m' | \frac{\mu}{z} | l, m \rangle$$

IF $l' \neq l$ AND $m' \neq m$

WE GET TO LOWEST APPROXIMATION

$$\begin{aligned}
\langle l', m' | \hat{z} | l, m \rangle &= \langle l', m' | r \cos \theta | l, m \rangle \\
&= r \langle l', m' | \cos \theta | l, m \rangle \\
&\sim r \langle l', m' | Y_1^0 | l, m \rangle \\
&= r \int_0^\pi \int_0^{2\pi} Y_{l'}^{m'}(\theta, \varphi) \left(Y_1^0(\theta, \varphi) Y_l^m(\theta, \varphi) \right) \sin \theta \, d\theta \, d\varphi
\end{aligned}$$

BUT

$$Y_1^0 Y_l^m \sim a Y_{l+1}^m + b Y_{l-1}^m$$

$$\begin{aligned}
\langle l', m' | \hat{z} | l, m \rangle &\sim a \langle l', m' | l+1, m \rangle + \\
&\quad b \langle l', m' | l-1, m \rangle
\end{aligned}$$

Integration over $\varphi \Rightarrow m' = m$

AND $\Delta l = \pm 1$ FOR ALLOWED TRANSITIONS

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \Psi}{\partial t^2} \quad \text{WAVE EQ.}$$

$$\Psi(x,t) = \phi(x) e^{i(2\pi\nu t)}$$

$$e^{i(2\pi\nu t)} \frac{d^2 \phi}{dx^2} = \frac{(i(2\pi\nu))^2}{v^2} e^{i(2\pi\nu t)} \phi$$

$$\textcircled{I} \quad v \rightarrow \frac{E}{\sqrt{2m(E-V)}}$$

OPTICS \longleftrightarrow CLASSICAL MECHANICS

$$e^{i(2\pi\nu t)} \frac{d^2 \phi}{dx^2} = - \frac{(2\pi)^2 \nu^2 [2m(E-V)]}{E^2} \phi e^{i(2\pi\nu t)} \quad \frac{h^2}{h^2}$$

$$\textcircled{II} \quad E = h\nu \Rightarrow \nu = \frac{E}{h}$$

$$e^{i\frac{E}{h}t} \frac{d^2 \phi}{dx^2} = - \frac{2m}{h^2} (E-V) \phi e^{i\frac{E}{h}t}$$

$$- \frac{h^2}{2m} \left[e^{i\frac{E}{h}t} \frac{d^2 \phi}{dx^2} \right] + V e^{i\frac{E}{h}t} \phi = E e^{i\frac{E}{h}t} \phi$$

$$= \frac{h}{i} \frac{\partial}{\partial t} \left[e^{i\frac{E}{h}t} \phi \right]$$

$$\boxed{- \frac{h^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V \Psi = \frac{h}{i} \frac{\partial \Psi}{\partial t}}$$

TISE

$$-\frac{\hbar^2}{2m} \frac{d^2 \phi}{dx^2} + V \phi = E \phi$$

$$(\hat{K} + \hat{V}) \phi = \hat{H} \phi = E \phi$$

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \hat{V}$$

FOR HYDROGEN ATOM

$$\hat{V}(r) = + \frac{ze^2 q}{4\pi\epsilon_0 r} = - \frac{ze^2}{4\pi\epsilon_0 r}$$

$$\hat{K} = -\frac{\hbar^2}{2\mu r^2} \frac{d}{dr} r^2 \frac{d}{dr} + \frac{1}{2I} L^2$$

$$\phi(r, \theta, \omega) = R(r) Y_l^m(\theta, \omega)$$

$$-\frac{\hbar^2}{2\mu r^2} \frac{d}{dr} \left[r^2 \frac{dR}{dr} \right] + \left[\frac{\hbar^2 l(l+1)}{2I} - \frac{ze^2}{4\pi\epsilon_0 r} \right] R = E R$$

$$E_n = - \frac{\mu |e|^4}{8\epsilon_0^2 \hbar^2} \frac{1}{n^2}$$

Hydrogenlike Atoms

$$\Psi_{nlm}(r, \theta, \phi) = R_{nl}(r) Y_l^m(\theta, \phi)$$

$$Y_l^m(\theta, \phi) = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_l^m(\cos \theta) e^{im\phi}$$

$$\int_0^{2\pi} \int_0^\pi Y_{l'}^{m'}(\theta, \phi) Y_l^m(\theta, \phi) \sin \theta d\theta d\phi = \delta_{l,l'} \delta_{m,m'}$$

FOR A GIVEN $n \rightarrow l=0, 1, 2, \dots, n-1$ AND $m=0, \pm 1, \dots, \pm l$
(Aufbau)

$$R_{nl}(r) = \sqrt{\left(\frac{2Z^3}{na_0}\right) \frac{(n-l-1)!}{2n[(n+l)!]}} (\alpha r)^l e^{-\alpha r/2}$$

$$\left\{ \begin{array}{l} 2l+1 \\ (\alpha r) \\ n-l-1 \end{array} \right.$$

$$\alpha = \frac{2Z}{na_0}$$

$$\int_0^\infty e^{-x} x^k \binom{k}{n} \binom{k}{m} dx = \frac{(n+k)!}{n!} \delta_{m,n}$$

$$\int_0^\infty e^{-x} x^{k+1} \binom{k}{n} \binom{k}{n} dx = \frac{(n+k)!}{n!} (2n+k+1)$$