Hydrogen atom, Coulomb potential w/ Schödinger eq:

→ results and basic ideas, derivation on other page.

$$\boxed{\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right]\Psi(\vec{r}) = E\Psi(\vec{r}) \qquad \vec{r} = (x,y,z),\ \nabla^2 = \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}}$$

↳ Coulombs law: $V(r) = -\frac{1}{4\pi\varepsilon_0}\cdot\frac{Ze^2}{r}$

Converted to spherical:

$$-\frac{\hbar^2}{2\mu}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\right]\Psi(r,\theta,\phi) + V(r)\Psi(r,\theta,\phi) = E\Psi(r,\theta,\phi)$$

becomes after $\hat{F}$ and $\hat{G}$

Solve PDE by seperation:

$\Psi(r,\theta,\phi) = R(r)\,Y(\theta,\phi)$

operates on Ψ *

* $\hat{G}(r) = -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + V(r)$ ← radial!

* $\hat{F}(\theta,\phi) = \frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$ ← angular! *

$$\hat{G}(r)\Psi(r,\theta,\phi) - \frac{\hbar^2}{2\mu r^2}\hat{F}(\theta,\phi)\Psi(r,\theta,\phi) = E\Psi(r,\theta,\phi)$$

Now splitting $Y = f(\theta)g(\phi)$:

$R(r)$: $\left[\frac{-\hbar^2}{2\mu}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) + \left(V(r) + \frac{\hbar^2}{2\mu r^2}\lambda\right)\right]R(r) = E(R(r))$

$f(\theta)$: $\left(\frac{d^2}{d\theta^2} + \cot\theta\frac{d}{d\theta} - \frac{m^2}{\sin^2\theta}\right)f(\theta) = -\lambda f(\theta)$ → $\lambda = l(l+1)$ l is angular ~~q~~ mentum #

$g(\phi)$: $\frac{d^2}{d\phi^2}g(\phi) = -m^2 g(\phi)$ → m is magnetic quantum #

↳ $g(\phi) = e^{im\phi}$

→ $\hat{F}(\theta,\phi)\,Y_{l,m}(\theta,\phi) = -l(l+1)\,Y_{l,m}(\theta,\phi)$ and $\boxed{Y_{l,m}(\theta,\phi) = f_{l,m}(\theta)\,e^{im\phi}}$ Spherical Harmonics

Angular Probability density: $P(\theta,\phi) = |Y_{l,m}(\theta,\phi)|^2$ ← no $\sin\theta$?

Radial Probability density: $P(r) = r^2|R_{nl}(r)|^2$ ← why r^2?

Normalization:

$$\int_{\text{all space}} P(r,\theta,\phi)\,dV = 1, \quad P(r,\theta,\phi)\,dV = |R(r)|^2|Y_{l,m}(\theta,\phi)|^2\,dV, \quad dV = r^2\sin\theta\,dr\,d\theta\,d\phi$$

Convention → $\int_0^\infty r^2|R(r)|^2\,dr = 1$, $\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}|Y_{l,m}(\theta,\phi)|^2\sin\theta\,d\theta\,d\phi = 1$

Radial sol'n: $R_{nl}(r) = C\left(\frac{Z}{na_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)^l\exp\left(-\frac{Zr}{na_0}\right)L_{nl}\left(\frac{Zr}{a_0}\right)$ associated Laguerre Polynomi

$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2}$, $E_n = \frac{-me^4}{32\pi^2\varepsilon_0^2\hbar^2}\left(\frac{Z^2}{n^2}\right)$

Expectation value of r:

$$\langle r\rangle = \int_0^\infty r\cdot r^2|R_{nl}(r)|^2\,dr\ \underbrace{\int_0^\pi\int_0^{2\pi}|Y_{l,m}(\theta,\phi)|^2\sin\theta\,d\phi\,d\theta}_{=1}$$

$= 1$ bec/ normalization condition.

↳ over full range = 1!

↳ u(x) reason why for r^2 ... $r^2|R(r)|^2$?

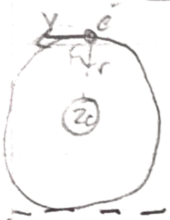
n = energy levels
l = orbital [illegible]
m = orientation, where it lays

Selection Rule and Angular momentum. $l = 0, 1, 2, 3, 4, \ldots$

→ if an electron wishes to change to a different orbital (s, p, d, f, g …) can only change by ± 1. $\boxed{\Delta l = \pm 1 \text{ and same for } m,\ \Delta m = 0, \pm 1}$

ex $1s \to 3p$ but $1s \not\to 3d$, n has no restriction, proof online, something w/ symmetry
($1s$: n, l)

Recall Bohr



quantization of angular momentum

$L = r \times p = mvr = n\hbar$, $r_n = \frac{4\pi\varepsilon_0 \hbar^2}{me^2}\frac{n^2}{Z^2} = a_0\frac{n^2}{Z^2}$, $E_n = \frac{-me^4}{32\pi^2\varepsilon_0^2\hbar^2}\frac{Z^2}{n^2}$ ← total energy

→ he got some right

Quantum angular momentum:

$\hat{p} = -i\hbar\frac{\partial}{\partial x}$, $r = \langle x, y, z \rangle$, $\nabla = \langle \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \rangle$

classical → $\hat{L} = \vec{r} \times \vec{p}$, QM → $\hat{L} = \hat{r} \times \hat{p} = \hat{r} \times (-i\hbar\nabla)$ (operator) ← now you can do whatever u want w/ these vectors.

projection of $\hat{L}$ onto z-axis:

$\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$ and $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$

↳ in spherical!

$\hat{L}^2 = -\hbar^2\left[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$, z-comp: $\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$

$\hat{L}^2 = -\hbar^2\hat{F}(\theta,\phi)$ $\hat{F}(\theta,\phi)$ + recall → * $\hat{F}(\theta,\phi)Y_{lm}(\theta,\phi) = -l(l+1)Y_{lm}(\theta,\phi)$ *

$\hat{F}(\theta,\phi) = \frac{\hat{L}^2}{-\hbar^2}$

plugging into!

$\boxed{\hat{L}^2 Y_{lm}(\theta,\phi) = l(l+1)\hbar^2 Y_{lm}(\theta,\phi)}$ ← solve same way like last time but we want z-comp for simplicity.

$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$ and $Y_{lm}(\theta,\phi) = f(\theta)g(\phi) = f(\theta)e^{im\phi}$ apply $\hat{L}_z$.

$\hat{L}_z Y_{lm}(\theta,\phi) = -i\hbar f(\theta)\frac{\partial}{\partial\phi}e^{im\phi} = m\hbar f(\theta)e^{im\phi} = m\hbar Y(\theta,\phi) = \hat{L}_z Y_{lm}(\theta,\phi)$

I don't know why.

For a $Y_{lm}(\theta,\phi)$ if we ↳ measure $|L|$ or L_z we get (using this for $|L|$) $\boxed{L^2 = l(l+1)\hbar^2 \text{ and } L_z = m\hbar}$ using this for L_z

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ex Find $|\vec{L}|$, L_z possible values, max + min value of $\langle \hat{L}_x^2 + \hat{L}_y^2 \rangle$ for $Y_{2m}(\theta,\phi)$. $l = 2$

$|\vec{L}| = \sqrt{l(l+1)}\hbar = \sqrt{6}\hbar$

$L_z = m\hbar$, $m = -2, -1, 0, 1, 2$ → $L_z = -2\hbar, -\hbar, 0, \hbar, 2\hbar$

⟨means⟩ expectation value → relates to magnitude? or the eigenvalues

$\langle \hat{L}^2 \rangle = \langle \hat{L}_z^2 \rangle + \langle \hat{L}_y^2 \rangle + \langle \hat{L}_x^2 \rangle$

$\langle \hat{L}_x^2 + \hat{L}_y^2 \rangle = -\langle \hat{L}_z^2 \rangle + \langle \hat{L}^2 \rangle = \hbar^2(l(l+1)) - m^2\hbar^2 = \hbar^2[l(l+1) - m^2]$

max at $m = 0$, $l = 2$ > $L_z = 6\hbar^2$

min at $m = -2\hbar^2$ or $+2\hbar^2$ idk

more Basic Notes Hydrogen Atom + Qm

magnitude only → $m = 2$, $l = 1$? or $-4\hbar^2$?

1, 7, 18, ?, 12, 15
1, 1, 7

$$\boxed{\int_0^\infty x^n e^{-cx}\,dx = \frac{n!}{c^{n+1}}}$$

Book Notes

Hydrogen Atom and Quantum Mechanics — bye bye Bohr

→ Our potential will be the Coulomb potential: $U(r) = \frac{-e^2}{4\pi\varepsilon_0 r}$

↳ one dimensional version:

x=0 • p+ ——— electron ——→ x

solve y_h, $y_p + y_h = 0$
y_p use variation of parameters
gets nasty integral
maybe Laplace transform makes it cake

7.2 $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) - \frac{e^2}{4\pi\varepsilon_0 x}\psi(x) = E\psi(x)$ ← solving this is doable but gross

↳ book solves it by constraining ODE with physics intuition

$\psi \xrightarrow{\text{must}} 0$ as $x \to \infty$, in order for $\frac{e^2}{4\pi\varepsilon_0}\cdot\frac{1}{x}\cdot\psi(x)$ you need $\psi(x) = 0$ at $x=0$, for no $\frac{1}{0}$

wave function that does this: $\psi(x) = Axe^{-bx}$, A is normalization constant

[→ taking derivatives + plugging in] → $b = \frac{me^2}{4\pi\varepsilon_0\hbar^2} = \frac{1}{a_0}$ ← bohr radius, $E = \frac{-\hbar^2 b^2}{2m}$, identical *by chance* to ground state of Bohr

Angular momentum

→ quantum thinks about angular momentum very differently. [Described by 2 quantum #'s, l, m_l]

(Bohr said $|\vec{L}| = n\hbar$)

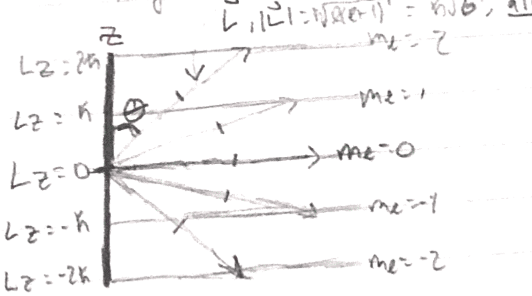
7.5 → length of $\vec{L}$ → $\boxed{|\vec{L}| = \hbar\sqrt{l(l+1)}}$ $l = 0, 1, 2, \ldots$

→ m_l, tells us about one component of the angular momentum vector

choose z, 7.6 $\boxed{L_z = m_l\hbar}$ $m_l = (0, \pm1, \pm2, \ldots, \pm l)$, for each value of l, there are $2l+1$ m_l's

~~angular momentum in 3D space only described w/ 2 numbers, needs a 3rd~~ but thats later

$\vec{L}$, $|\vec{L}| = \hbar\sqrt{l(l+1)} = \hbar\sqrt{6}$, all same length



7.7 $\cos\theta = \frac{L_z}{|\vec{L}|} = \frac{m_l}{\sqrt{l(l+1)}}$

ex] $l = 1$ → $m_l = -1, 0, +1$

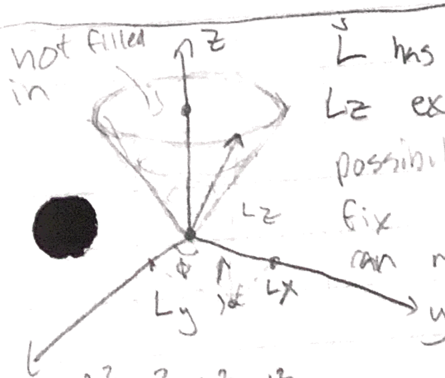
$L_z = m_l\hbar$ → $L_z = -\hbar, 0, \hbar$

$|\vec{L}| = \hbar\sqrt{2}$

$\cos\theta = \frac{-\hbar, 0, \hbar}{\hbar\sqrt{2}} = -\frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}}$

$\theta = 45°, 90°, 135°$, only certain angles!

not filled in



$|\vec{L}|^2 = L_x^2 + L_y^2 + L_z^2$

$\vec{L}$ has 3 components, if we know L_z exactly then theres many possibility for L_x and L_y.

fix L_z but L_x, L_y can make it form a cone, cone represents all possible combos for $L_x + L_y$

→ uncertainty in L_x, L_y for L_z

$\Delta L_z \Delta\phi \geq \hbar$, if we know L_z exactly, cant know ϕ at all

$L_z < |L|$ unless $l = 0$

Hydrogen Atom Wave Function

Cartesian: $-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}\psi + \frac{\partial^2}{\partial y^2}\psi + \frac{\partial^2}{\partial z^2}\psi\right) + U(x,y,z)\psi(x,y,z) = E\psi(x,y,z)$

Usual method is to have $\psi(x,y,z) = X(x)\,Y(y)\,Z(z)$ but coulomb doesn't seperate has $\boxed{\sqrt{x^2+y^2+z^2}}$ ← hints to use spherical coordinates (r,θ,ϕ)

7.10

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial r^2} + \frac{2}{r}\frac{\partial\psi}{\partial r} + \frac{1}{r^2\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right] + U(r)\psi(r,\theta,\phi) = E\psi(r,\theta,\phi)$$

Now its seperable w/ $\psi(r,\theta,\phi) = R(r)\,\Theta(\theta)\,\Phi(\phi)$

polar & azimuthal sol'n are combos of trig func

quantum state of a particle that moves in a potential that only depends on r, $U(r)$ can be described by l and m_l

radial: $-\frac{\hbar^2}{2m}\left(\frac{d^2R}{dR^2} + \frac{2}{r}\frac{dR}{dr}\right) + \left(\frac{-e^2}{4\pi\varepsilon_0 r} + \frac{l(l+1)\hbar^2}{2mr^2}\right)R(r) = E\,R(r)$

↑ reduced mass of proton-electron system

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like n, when solving Schrodinger eq in 3 dimensions 3 numbers emerge from sol'n w/ hydro wave func (pg 204)

n = principle quantum # = 1, 2, 3...

l = angular momentum Q# = 0, 1, 2, ..., n-1

m_l = magnetic Q# = 0, ±1, ±2, ±l

n comes from, determining quantized energy levels

$E_n = \frac{-me^4}{32\pi^2\varepsilon_0^2\hbar^2}\cdot\frac{1}{n^2}$, Energy depends only on n

→ (n, l, m_l) the seperated can be written now as: $\psi_{n,l,m_l}(r,\theta,\phi) = R_{n,l}(r)\,\Theta_{l,m_l}(\theta)\,\Phi_{m_l}(\phi)$

Probability Densities

prob density = $|\psi(r,\theta,\phi)|^2$ ∴ to find probability in a region of space: $\int|\psi(r,\theta,\phi)|^2\,dV$, $dV = r^2\sin\theta\,dr\,d\theta\,d\phi$

therefore prob of particle e → $|\psi_{n,l,m_l}(r,\theta,\phi)|^2 dV = \int\int\int |R_{n,l}(r)|^2\,|\Theta_{l m_l}(\theta)|^2\,|\Phi_{m_l}(\phi)|^2\,r^2\sin\theta\,dr\,d\theta\,d\phi$ [complete probability density to locate an e]

---

instead lets find the probability at certain distance. → [whats prob of finding e between spheres of r, r+dr] → radial prob density, prob within that shell. $P(r)$, $P(r)dr$

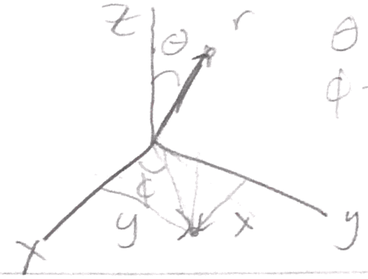
$P(r)dr = |R_{nl}(r)|^2 r^2 dr \int_0^{\pi}|\Theta_{l m_l}(\theta)|^2\sin\theta\,d\theta\int_0^{2\pi}|\Phi_{m_l}(\phi)|^2 d\phi$, both $\Phi, \Theta = 1$ when normalized ← not sure exactly

$P(r) = r^2|R_{nl}(r)|^2$

$P(\theta,\phi) = |Y_{l,m}(\theta,\phi)|^2$

Hydrogen atom sol'n, quantum #'s derivation

Physics Notes



$\theta = 0 \to \pi$
$\phi = 0 \to 2\pi$

Schrodinger in spherical coordinates!

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\left(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\right]\psi(r,\theta,\phi)+V(r)\psi(r,\theta,\phi)=E\psi(r,\theta,\phi)$$

try to seperate! then use seperated,

by

$$\psi(r,\theta,\phi)=R(r)\,Y(\theta,\phi)$$

plug in

$$\boxed{\begin{aligned}\hat{G}(r) &= -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right)+V(r)\\ \hat{F}(\theta,\phi) &= \frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\end{aligned}}$$

rewrite w/ these

$$\hat{G}(r)\psi(r,\theta,\phi)-\frac{\hbar^2}{2mr^2}\hat{F}(\theta,\phi)\psi(r,\theta,\phi)=E\psi(r,\theta,\phi)$$

$$\hat{G}(r)R(r)Y(\theta,\phi)-\frac{\hbar^2}{2mr^2}\hat{F}(\theta,\phi)R(r)Y(\theta,\phi)=E\,R(r)Y(\theta,\phi)$$

divide over

$$\frac{1}{R(r)}\hat{G}(r)R(r)-\frac{\hbar^2}{2mr^2}\cdot\underbrace{\frac{1}{Y(\theta,\phi)}\hat{F}(\theta,\phi)Y(\theta,\phi)}_{-\lambda}=E$$

$$\boxed{\begin{aligned}&\text{Angular: } \frac{1}{Y(\theta,\phi)}\hat{F}(\theta,\phi)Y(\theta,\phi)=-\lambda=\text{constant}\\ &\text{Radial: } \frac{1}{R(r)}\hat{G}(r)R(r)+\frac{\hbar^2}{2mr^2}\lambda=E\end{aligned}}$$

plugged $\hat{F}$ in

Angular seperation of: $\frac{\partial^2}{\partial\theta^2}Y(\theta,\phi)+\cot\theta\frac{\partial}{\partial\theta}Y(\theta,\phi)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}Y(\theta,\phi)=-\lambda Y(\theta,\phi)$

sub $Y(\theta,\phi)=f(\theta)g(\phi)$

$$\frac{\partial^2}{\partial\theta^2}f(\theta)g(\phi)+\cot\theta\frac{\partial}{\partial\theta}f(\theta)g(\phi)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}f(\theta)g(\phi)=-\lambda f(\theta)g(\phi)$$

divide over

$$\frac{1}{f(\theta)}\frac{\partial^2}{\partial\theta^2}f(\theta)+\frac{1}{f(\theta)}\cot\theta\frac{\partial}{\partial\theta}f(\theta)+\frac{1}{\sin^2\theta}\underbrace{\frac{1}{g(\phi)}\frac{\partial^2}{\partial\phi^2}g(\phi)}_{\phi\text{ stuff }=-m^2}=-\lambda$$

magnetic quantum num

Polar: $\left(\frac{d^2}{d\theta^2}+\cot\theta\frac{d}{d\theta}-\frac{m^2}{\sin^2\theta}\right)f(\theta)=-\lambda f(\theta)$

Azimuthal: $\frac{d^2}{d\phi^2}g(\phi)=-m^2g(\phi)$

then $\longrightarrow$

$\psi(r,\theta,\phi) = R(r)f(\theta)g(\phi)$

$R(r)$: $\left[-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) + \left(U(r) + \frac{\hbar^2}{2mr^2}\lambda\right)\right]R(r) = E\,R(r)$ solve this for E?

$f(\theta)$: $\left(\frac{d^2}{d\theta^2} + \cot\theta\frac{d}{d\theta} - \frac{m^2}{\sin^2\theta}\right)f(\theta) = -\lambda f(\theta)$ for λ

$g(\phi)$: $\frac{d^2}{d\phi^2}g(\phi) = -m^2 g(\phi)$ solve for m to solve

can solve,

$g(\phi) = e^{im\phi}$ ϕ can be 0 to 2π and change by 0 or 2π shouldn't change wave function

$g(\phi) = g(\phi + 2\pi) \rightarrow \exp(im\phi)\exp(im2\pi) = \exp(im\phi)$

$\boxed{\exp(im2\pi) = 1}$ $m = 0, \pm 1, \pm 2,$ magnetic quantum num

now solving $f(\theta)$

$\left(\frac{d^2}{d\theta^2} + \cot\theta\frac{d}{d\theta} - \frac{m^2}{\sin^2\theta}\right)f(\theta) = -\lambda f(\theta)$ eigenfunctions are called associated Legendre functions

Legendre function solutions only exist for $\boxed{\lambda = \ell(\ell+1)}$ $\ell = 0, 1, 2, \ldots$

ℓ is angular quantum number and $f_{\ell m}(\theta)$,

thus $m = -\ell, -(\ell-1), \ldots 0 \ldots, \ell-1, \ell$ goes from $-\ell$ to ℓ

$\boxed{Y_{\ell m}(\theta,\phi) = f_{\ell m}(\theta)e^{im\phi}}$ (Spherical Harmonics)

$F(\theta,\phi)\,Y_{\ell m}(\theta,\phi) = -\ell(\ell+1)\,Y_{\ell m}(\theta,\phi)$

Physics Notes

$$\Psi(r,\theta,\phi) = R(r)\, Y_{\ell m}(\theta,\phi)$$

(radial) (Spherical Harmonics)

[Probability of finding the é] $\rightarrow$ $P(r,\theta,\phi)\,dV = |R(r)|^2 |Y_{\ell m}(\theta,\phi)|^2\, dV$

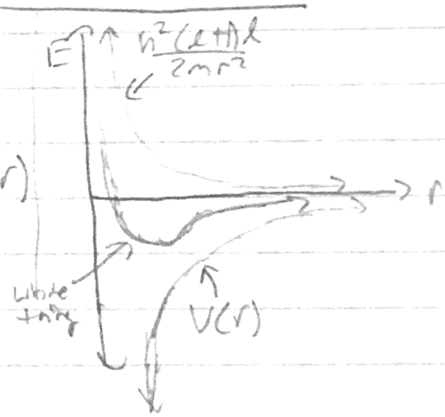
[Normalization] $\rightarrow$ $\int_{\text{all space}} r^2 P(r,\theta,\phi)\, dV = 1$ $\qquad dV = r^2 dr \sin\theta\, d\theta\, d\phi$

Radial: $\int_0^\infty r^2 |R(r)|^2\, dr = 1$

Angular: $\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi} |Y_{\ell m}(\theta,\phi)|^2 \sin\theta\, d\theta\, d\phi = 1$

Finally for Radial Solution

$$-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)R(r) + \underbrace{\left[V(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}\right]}_{\text{effective potential energy}} R(r) = E R(r)$$



$$R_{n\ell} = C\left(\frac{Z}{na_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)^{\ell} \exp\left(-\frac{Zr}{na_0}\right) L_{n\ell}(Zr/a_0)$$

$\uparrow$ exponent $\qquad \uparrow$ Laguerre polynomial

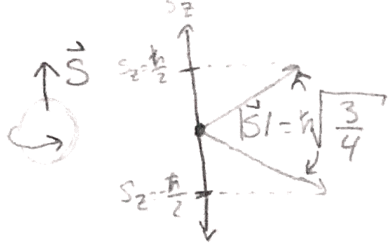
$$E_n = \frac{-me^4}{32\pi^2\varepsilon_0^2\hbar^2}\frac{Z^2}{n^2}$$

$R_{10}(r) = 2\left(\frac{Z}{a_0}\right)^{3/2} \exp(-Zr/a_0)$

$R_{20}(r) = 2(Z/2a_0)^{3/2}(1 - Zr/2a_0)\exp(-Zr/2a_0)$

Radial Prob density!

norm cond $\int_0^\infty r^2 |R_{n\ell}(r)|^2 dr = 1$, $P(r) = R_{n\ell}^2(r)\, r^2$



Spin - intrinsic angular momentum

Spin doesn't enter Schrödinger eq. but is in Dirac's relativistic QM

Orbital angular momentum:

- $\to \vec{L}$ has $\vec{L}_x, \vec{L}_y, \vec{L}_z$
- $l = 0, 1, 2, \ldots$
- $\to (L_z) Y_{l,m_l}(\theta,\phi) = (m_l \hbar) Y_{l,m_l}(\theta,\phi)$
- $\to m_l = -l, \ldots l$
- $\to \vec{\mu}_l = -\frac{e}{2m_e}\vec{L}$ (mass of electron)
- $\to \vec{L}^2 Y_{l,m_l}(\theta,\phi) = l(l+1)\hbar^2 Y_{l,m_l}(\theta,\phi)$

forgot

Spin - intrinsic angular momentum

- $\to \vec{S}$ has $\vec{S}_x, \vec{S}_y, \vec{S}_z$
- $\to \vec{S}^2 = s(s+1)$
- $s = \frac{1}{2}$
- $\to S_z = m_s \hbar$
- $\to m_s = -s, \ldots s \to \pm\frac{1}{2}$
- $\to \vec{\mu}_s = -\frac{e}{m_e}\vec{S}$

$\vec{S}$ works almost identical to $\vec{L}$ excepts Q# is always $\frac{1}{2}$ for example

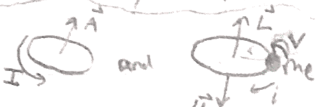
Value of $\langle \hat{S}_x^2 + \hat{S}_y^2 \rangle = \langle \hat{S}^2 \rangle - \langle \hat{S}_z^2 \rangle = \begin{pmatrix} \text{plug in} \\ s = \frac{1}{2} \\ m_s = \frac{1}{2} \end{pmatrix} = \frac{\hbar^2}{2}$

$\langle \hat{S}^2 \rangle \to s(s+1)\hbar^2$, $\langle \hat{S}_z^2 \rangle \to (m_s\hbar)^2$

note: $\langle \hat{S}^2 \rangle = \int \psi^* \hat{S}^2 \psi \, dV$

Magnetic dipole moment:

Recall: $\vec{\mu} = I\vec{A}$



$I = \frac{e}{T}$ (e positive), $T = \frac{2\pi r}{v}$, $I = \frac{ev}{2\pi r}$, $\vec{\mu}_L = (-\hat{z}) I A = -\frac{evr}{2}\hat{z}$, $A = \pi r^2$, $\vec{L} = \vec{r} \times \vec{p} = m_e v r \hat{z}$ finished on first

Classically: $\frac{\vec{\mu}_L}{\vec{L}} = -\frac{e}{2m_e} \to \vec{\mu}_L = -\frac{e}{2m_e}\vec{L}$

Quantum mechanically:

Orbital Magnetic Dipole Moment

use: $\mu_L = -\frac{e}{2m_e}\vec{L}$, $\underset{\text{magnitude}}{\mu_{L,z}} = -\frac{e}{2m_e} L_z = -\frac{e\hbar}{2m_e} m_l = \boxed{-\mu_B m_l}$

$L_z = m_l \hbar$, $\frac{e\hbar}{2m_e}$: Bohr magneton

Spin Magnetic Dipole Moment

$\vec{\mu}_s = -\frac{e}{m_e}\vec{S}$, $\mu_{s,z} = -\frac{e}{2m_e} S_z$, $S_z = m_s \hbar$

$\mu_{s,z} = -\frac{e}{m_e} m_s \hbar = \boxed{-2m_s \mu_B = \mu_{L,z}}$

Stern-Gerlach Experiment!

↙ orientation

→ A beam of H is $n=2, l=1$ state, $\underline{m_l = -1, 0, 1}$
→ beam pass through a non uniform magnetic field

↙ why not other way?

$m_l = 1 \rightarrow \mu_{l,z} = -\mu_B m_l = -\mu_B$ get deflected **up**
$m_l = -1$ get deflected down
$m_l = 0$ are undeflected

<u>when doing experiment:</u>
→ We find not 3 images but 6 images!
→ if done with $l=0$ state we would see 2 images!
↳ in $l=0$ we expect $\vec{L}$ has length $=0$ $\left(|L^2| = l(l+1)\hbar^2\right)$

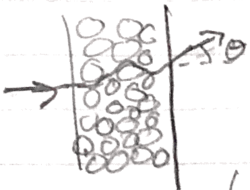
<u>In general:</u>
expected 2 images, one for + and −, and the 0
↳ so $2l+1$ images
But with $l=0$ we got 2 images so $l = 1/2$.
↳ not permitted by Schrödinger eq so we add another Q# to contribute to the angular momentum, spin.

$S = \frac{1}{2}$ quantum number s

$\vec{S}$ = angular momentum vector

Mutheford
d
Tompson

~~BOHR Stuff~~

[Thomson scattering prediction] →  random walk (can only go up or down)

Number of atoms thru k.

$\Theta \simeq \sqrt{N}\,\Theta_{ave}$ (small angles only)

↳ large angles dont fit model,

↝ thompson said its like plum pudding

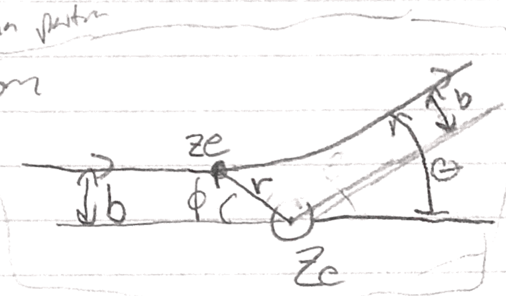
↝ but density matters, atoms mostly "empty space"

↓

[Mutheford]

alpha particle

$F = \frac{1}{4\pi\varepsilon_0}\frac{(ze)(Ze)}{r^2}$ ← atom



main eq

$\frac{1}{r} = \frac{1}{b}\sin\phi + \frac{zZe^2(\cos\phi - 1)}{8\pi\varepsilon_0 b^2 K}$

↑ hyperbola in polar coordinates

↑ kinetic energy of particle

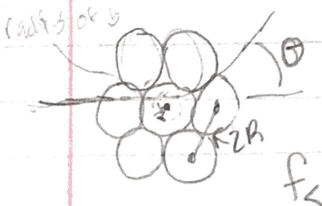
• Θ_{av} = after lots of approximations = $\frac{zZe^2}{16\pi\varepsilon_0 RK}$

→ using main eq, see what happens to b at $r = \infty$, this will tell you what its scattered angle is, also $180° = \Theta + \phi$ so $\phi = \pi - \Theta$

• $b = \frac{zZe^2}{8\pi\varepsilon_0 K}\cot\left(\frac{\Theta}{2}\right) = \frac{zZ}{2K}\cdot\frac{e^2}{4\pi\varepsilon_0}\cot\left(\frac{\Theta}{2}\right)$, as b increases Θ decreases, as b decreases Θ increases

by this stuff

$f_{<b} = f_{>\Theta}$ fraction of particles coming in w/ r less than b is the same fraction of particles w/ an angle greater than Θ,



$f_{<b} = \frac{\pi b^2}{\pi R^2}$ Radius between atomic nuclei, whats the Area of each atom?

consider a foil w/ thickness t, Area A, density ρ, molar mass M

$n = \frac{\#\text{ of particles}}{m^3} = \frac{\rho N_A}{M}$ → $\frac{g}{m^3}\cdot\frac{1\,mol}{g}\cdot\frac{6.022\times10^{23}\text{ particles}}{mol} = \frac{\text{Particles}}{m^3}$

ρ, $\frac{1}{M}$, $M = g/mol$, N_A

$nt = \frac{\#\text{ particles}}{m^2} = \frac{\rho N_A}{M}t$

[we want Area per Particle] $\frac{1}{nt} = \frac{m^2}{\#\text{ particles}} = \frac{\text{Area}}{1\text{ particle}} = \pi R^2$

might think its total but its density so you can plug in 1 particle

thus →

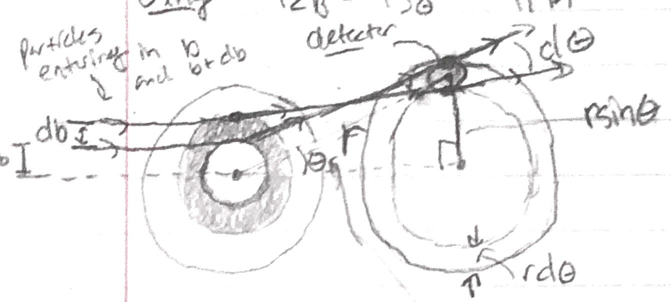
pg 2

Since

fraction of particles greater than θ

$n = \frac{\rho N_A}{M}$, $\frac{1}{nt} = \pi R^2$, $f_{>\theta} = f_{<b} = \frac{\pi b^2}{\pi R^2}$ (Area of incident particles) (total)

using $f_{<b} = f_{>\theta} = \frac{\pi b^2}{\pi R^2} = nt\pi b^2$



how many particles in the db and $d\theta$ go through the detector,

↓

whats fraction of particles go through that Area (detector) $\frac{df_{>\theta}}{dA}$

$f_{>\theta} = nt\pi b^2 \rightarrow df_{>\theta} = 2nt\pi b\, db$

$dA = (2\pi(r\sin\theta))(r\,d\theta)$ → (strip $rd\theta$ traces out) • (circumfrence of big circle) = small area traced out = dA

(circumfrence of big circle) (w/ that r see what changing by $d\theta$ does)

$b = \frac{zZ}{2K}\frac{e^2}{4\pi\varepsilon_0}\cot\left(\frac{\theta}{2}\right) \rightarrow db = \left(\frac{zZ}{4K}\right)\left(\frac{e^2}{4\pi\varepsilon_0}\right)\frac{1}{\sin^2(\theta/2)}d\theta$

$N(\theta) = \begin{pmatrix}\text{\# of particles}\\ \text{scattered thru}\\ \text{angle } \theta\end{pmatrix} = \frac{df}{dA} = \frac{(2nt\pi b)\left(\frac{zZ}{4K}\cdot\frac{e^2}{4\pi\varepsilon_0}\cdot\frac{1}{\sin^2(\frac{\theta}{2})}d\theta\right)}{(2\pi r^2\sin\theta\, d\theta)}$

all θ or just at θ? →

twice as 2K

$N(\theta) = \frac{nt}{4r^2}\left(\frac{zZ}{2K}\right)^2\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\frac{1}{\sin^4(\frac{\theta}{2})}$

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highlights

How close can an alpha particle get? Means $b=0$,

$K = \frac{1}{2}mV^2$ which has to equal $F \cdot d = \frac{zZe^2}{4\pi\varepsilon_0}\cdot\frac{1}{d}$

$\longrightarrow |\!\!-d-\!\!\oplus$

Energy & min dist

$$PE = U = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r^2} = \frac{1}{4\pi\varepsilon_0}\left(\frac{zZe^2}{r}\right)$$

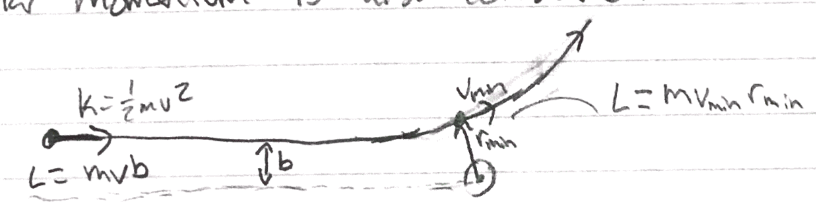
→ max potential energy occurs at min KE, think about a ball in air,
→ min radius occurs at max potential energy, where its closest too nucleus

starts w/

$K = \frac{1}{2}mv^2$ as it approaches $K\downarrow$ and $U\uparrow$ but $U+K=$ constant

- $$\underbrace{\frac{1}{2}mv_{min}^2}_{K_{min}} + \underbrace{\frac{1}{4\pi\varepsilon_0}\frac{zZe^2}{r_{min}}}_{U_{max}} = \underbrace{\frac{1}{2}mv^2}_{\text{All energy}}$$

- angular momentum is also conserved:



so $mvb = mv_{min}r_{min} \rightarrow v_{min} = \frac{bv}{r_{min}}$ sub in

$$\frac{1}{2}mv^2 = \frac{1}{2}m\left(\frac{b^2v^2}{r_{min}^2}\right) + \frac{1}{4\pi\varepsilon_0}\frac{zZe^2}{r_{min}}$$

Lyman series

n^{th} orbital electron speed

shortest & longest λ & lyman

Emission lines of hydrogen in visible region!

$$\lambda = (364.5\text{ nm})\frac{n^2}{n^2-4} \quad (n=3,4,5,\ldots)$$

n=3 corresponds to the longest λ of the series of hydrogen lines in visible

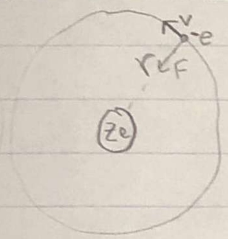
all groupings of lines in hydrogen spectrum could be fit like this

$$\lambda = \lambda_{limit}\frac{n^2}{n^2-n_0^2} \quad \cancel{(n = n_0+1, n_0+2, n_0+3, \ldots)}$$

λ_{limit} is the wavelength of the appropriate series limit,

(Lyman $n_0=1$) (Balmer $n_0=2$) (Paschen $n_0=3$) (Brackett $n_0=4$) (Pfund $n_0=5$)

BOHR MODEL



$$F = \frac{1}{4\pi\varepsilon_0}\frac{|q_1 q_2|}{r^2} = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{r^2} = \frac{mv^2}{r}$$

manipulating

$$K = \frac{1}{2}mv^2 = \frac{1}{8\pi\varepsilon_0}\frac{e^2}{r}$$

Coulomb Potential Energy $U = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r} = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}$

$$E_{tot} = K + U = \frac{1}{8\pi\varepsilon_0}\frac{e^2}{r} + \left(-\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r}\right) = -\frac{1}{8\pi\varepsilon_0}\frac{e^2}{r}$$

→ Bohr said angular momentum to integer "stationary states" so it fits classical theory,

↳ $\hbar, 2\hbar, 3\hbar$, etc... quantization of Angular Momentum

Subbing r_n into E_{tot}

$\vec{L} = \vec{r}\times\vec{p}$ has magnitude $L = rp = mvr$ when $r \perp \vec{p}$

$\boxed{mvr = n\hbar}$ → $\frac{1}{2}mv^2 = \frac{1}{2}m\left(\frac{n\hbar}{mr}\right)^2 = \frac{1}{8\pi\varepsilon_0}\frac{e^2}{r}$

thus $r_n = \frac{4\pi\varepsilon_0\hbar^2}{me^2}n^2 = a_0 n^2 \quad (n=1,2,3,\ldots)$ Bohr radius $a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = .0529\text{ nm}$

$$E_n = -\frac{me^4}{32\pi^2\varepsilon_0^2\hbar^2}\cdot\frac{1}{n^2} = \frac{-13.60\text{ eV}}{n^2} \quad (n=1,2,3,\ldots)$$

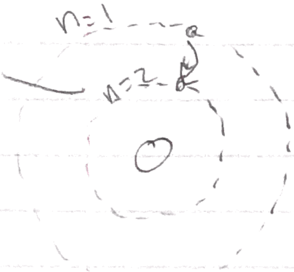
n=1 is ground state

ex

$\Delta E = E_2 - E_1 = -3.4 + 13.6 = 10.2\text{ eV}$,

$|E_n|$ = binding energy, if an atom absorbs that amount of energy the e^- will be removed,

Hydrogen wavelengths in Bohr model



if it goes from $n=1$ to $n=2$ and emits light

$hf = E_{n_1} - E_{n_2}$ if you use $E_n = -\frac{me^4}{32\pi^2\varepsilon_0^2\hbar^2}\frac{1}{n^2}$ for energies

$$f = \frac{me^4}{64\pi^3\varepsilon_0^2\hbar^3}\left(\frac{1}{n_2^2} - \frac{1}{n_1^2}\right)$$ and $\lambda = \frac{c}{f}$ so

$$\lambda = \frac{64\pi^3\varepsilon_0^2\hbar^3 c}{me^4}\left(\frac{n_1^2 n_2^2}{n_1^2 - n_2^2}\right) = \frac{1}{R_\infty}\left(\frac{n_1^2 n_2^2}{n_1^2 - n_2^2}\right)$$

R_∞ = Rydberg constant
$R_\infty = 1{,}0973{,}1 \cdot 10^7\ m^{-1}$

→ Atoms with charge $Z > 1$, any atom w/ a single electron, ex ionized helium, doubly ionized lithium etc..

$$F = \frac{1}{4\pi\varepsilon_0}\frac{q_1 q_2}{r^2} = \frac{1}{4\pi\varepsilon_0}\frac{Ze^2}{r^2}$$ ← nucleus of charge Ze the Coulomb force acting on it is,

only Z change so:

$$r_n = \frac{4\pi\varepsilon_0\hbar^2}{Ze^2 m}n^2 = \frac{a_0 n^2}{Z}, \quad E_n = \frac{-m(Ze^2)^2}{32\pi^2\varepsilon_0^2\hbar^2}\cdot\frac{1}{n^2} = -(13.60\,eV)\frac{Z^2}{n^2}$$