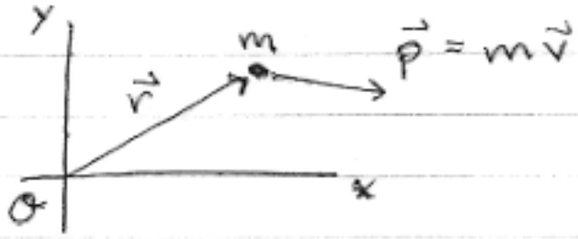
Angular Momentum (warm-up for H-atom)

Classically, angular momentum defined as (for a 1-particle system)

$$\vec{L} \equiv \vec{r} \times \vec{p}$$

$$= \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$



Note: $\vec{L}$ defined w.r.t. an origin of coords

$$\vec{L} = \hat{x}(y p_z - z p_y) + \hat{y}(z p_x - x p_z) + \hat{z}(x p_y - y p_x)$$

(In QM, the operator corresponding to L_x is

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \quad p_z = \frac{\hbar}{i}\frac{\partial}{\partial z}, \text{ etc.}$$

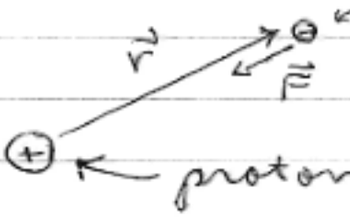
~ according to prescription of Postulate 2, part 3)

Classically, torque defined as $\vec{\tau} \equiv \vec{r} \times \vec{F}$, and

$$\vec{\tau} = \frac{d\vec{L}}{dt}$$ (rotational version of $\vec{F} = m\vec{a}$)

If the force is radial (central force), then $\vec{\tau} = \vec{r} \times \vec{F} = 0 \Rightarrow \vec{L} = \text{const}$

H-atom:



In a multi-particle system, total ang. mom.

$\vec{L}_{tot} = \sum_i \vec{L}_i$ is conserved for system isolated from external torques

↖ sum over parts

Internal torques can cause exchange of ang. mom. among particles, but $\vec{L}_{tot}$ remains constant.

In classical and quantum mechanics, only 4 things are conserved:

- energy
- linear momentum
- angular momentum
- electric charge

Back to QM. Define vector operator $\hat{\vec{L}}$

$$\hat{\vec{L}} = \hat{L}_x \hat{x} + \hat{L}_y \hat{y} + \hat{L}_z \hat{z}$$

($\hat{}$ ← operator; $\hat{x}, \hat{y}, \hat{z}$ ← unit vector)

Recall $\frac{d\langle Q \rangle}{dt} = \frac{i}{\hbar} \langle [\hat{H}, \hat{Q}] \rangle$

$$\Rightarrow \underbrace{\frac{d\langle \hat{\vec{L}} \rangle}{dt}}_{\frac{d\langle L_x \rangle}{dt}\hat{x} + \frac{d\langle L_y \rangle}{dt}\hat{y} + \dots} = \frac{i}{\hbar} \langle [\hat{H}, \hat{\vec{L}}] \rangle$$

Claim: for a central force such as in H-atom

$V = V(r) = -ke^2/r$, then $[\hat{H}, \hat{\vec{L}}] = 0$

(will show this later)

This implies $\frac{d\langle \vec{L} \rangle}{dt} = 0$ (just like in classical mech.)

Angular momentum of electron in H-atom is constant, so long as it does not absorb or emit photon. Throughout present discussion, we ignore interaction of H-atom w/ photons.

Will show that for H-atom or for any atom, molecule, solid - any collection of atoms - the angular momentum is quantized in units of $\hbar$. $|\vec{L}|$ can only change by integer nbr of $\hbar$'s

units of $L = [L] = [\hbar]$

Note $[L] = [r\,p]$, $[p] = \left[\frac{\hbar}{r}\right]$ (since $p = \hbar k$)

$$\Rightarrow [L] = [r] \times [\hbar]/[r] = [\hbar] \quad \checkmark$$

Claim: $[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$

and $\boxed{[\hat{L}_i, \hat{L}_j] = i\hbar \hat{L}_k}$ (i, j, k cyclic: x y z or y z x or z x y).

To prove, need two very useful identities:

$$[A+B, C] = [A, C] + [B, C]$$

$$[AB, C] = A[B, C] + [A, C]B$$

Proof: $[L_x, L_y] = [y p_z - z p_y,\ z p_x - x p_z] =$

$[y p_z, z p_x] - [y p_z, x p_z] - [z p_y, z p_x] + [z p_y, x p_z]$

$y[p_z, z]\,p_x$ ($-i\hbar$) — all other terms like $[y, p_x] = 0$ — $x[z, p_z]\,p_y$ ($+i\hbar$)

$= +i\hbar(x p_y - y p_x) = i\hbar L_z$ ✓

(Have used $[x, p_x] = i\hbar$, $[x, y] = 0$, $[x, p_y] = 0$, $[p_x, p_y] = 0$, etc.)

I'm dropping the ^ over operators when no danger of confusion.

Since $[L_x, L_y] \neq 0$, cannot have simultaneous eigenstates of $\hat{L}_x$ and $\hat{L}_y$

$$\sigma^2_{L_x}\,\sigma^2_{L_y} \geq \left(\frac{1}{2i}\langle \underbrace{[\hat{L}_x, \hat{L}_y]}_{i\hbar\langle \hat{L}_z\rangle}\rangle\right)^2 = \left(\frac{\hbar}{2}\right)^2 \langle L_z\rangle^2$$

However, $L^2 = \vec{L}\cdot\vec{L} = L_x^2 + L_y^2 + L_z^2$ does commute w/ L_z

Claim: $[L^2, L_z] = 0$

$$\boxed{[L^2, L_i] = 0}, \quad i = x, y, \text{ or } z$$

Proof: $[L^2, L_z] = [L_x^2, L_z] + [L_y^2, L_z] + \underbrace{[L_z^2, L_z]}_{0}$

$= L_x\underbrace{[L_x, L_z]}_{-i\hbar L_y} + \underbrace{[L_x, L_z]}_{-i\hbar L_y}L_x + L_y\underbrace{[L_y, L_z]}_{+i\hbar L_x} + \underbrace{[L_y, L_z]}_{+i\hbar L_x}L_y$

$= 0$ (Note cancellations)

$[L^2, L_z] = 0 \Rightarrow$ can have simultaneous eigenstates of $\hat{L}^2$, $\hat{L}_z$ (or $\hat{L}^2$, $\hat{L}_i$ any i)

Looking forward to H-atom:

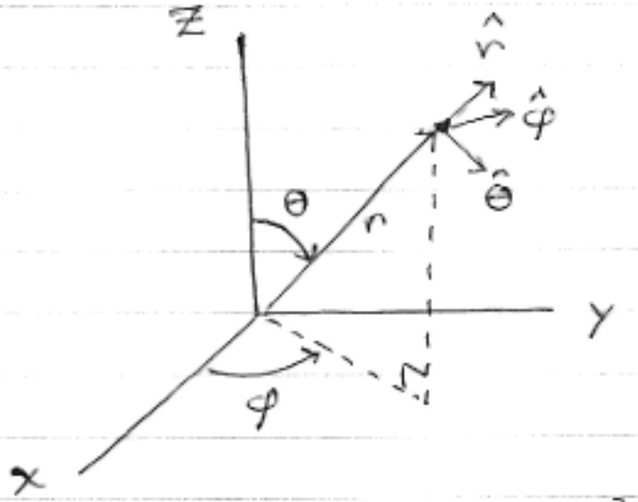
$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2(\,) + V(r)\cdot(\,)$$

We will show that $[\hat{H}, \hat{L}^2] = 0$, $[\hat{H}, \hat{L}_z] = 0$

$\Rightarrow$ simultaneous eigenstates of $\hat{H}$, $\hat{L}^2$, $\hat{L}_z$

$\psi = \psi_{n\,l\,m}$ ← energy q-nbr; m ← L_z q-nbr; l ← L^2 q-nbr

When we solve the TISE $\hat{H}\Psi = E\Psi$ for the H-atom, the natural coords to use will be spherical coords: r, θ, φ (not x, y, z)



$$x = r\sin\theta\cos\varphi$$
$$y = r\sin\theta\sin\varphi$$
$$z = r\cos\theta$$

Just rewriting $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ in spherical coords is gawd-awful. But separation of variables will give special solutions, ~~eqg~~ energy eigenstates, of form

$$\Psi(r,\theta,\varphi) = R(r)\,Y(\theta,\varphi) = R(r)\,\Theta(\theta)\,\Phi(\varphi)$$

the angular part of the solution $Y(\theta,\varphi)$ will turn out to be eigenstates of L^2, L_z and will have form completely independent of the potential $V(r)$.

Given only $[L^2, L_z] = 0$ and $\hat{L}^2, \hat{L}_z$ hermitean we know there must exist simultaneous eigenstates f (which will turn out to be the $Y(\theta,\varphi)$ mentioned above) such that

$$\hat{L}^2 f = \lambda \cdot f \quad , \quad \hat{L}_z f = \mu \cdot f$$

(λ will be related to l, μ will be related to m)

We will show that f will depend on quantum-nbrs l, m, so we write it as f_l^m, and that

$$L^2 f_l^m = \hbar^2 l(l+1) \cdot f_l^m$$

$$L_z f_l^m = \hbar m \cdot f_l^m$$

where $l = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$ $\quad m = -l, -l+1, \ldots l-1, l$

$f_l^m = Y_l^m(\theta, \varphi)$ will be determined later

Notice max eigenvalue of L_z ($= l\hbar$) is smaller than square root of eigenval of $L^2 = \hbar\sqrt{l(l+1)}$

So, in QM $L_z < |L|$ Odd!

Also notice $l = 0$, $m = 0$ state has zero angular momentum ($L^2 = 0$, $L_z = 0$) so, unlike Bohr model, can have electron in state that is "just sitting there" rather than revolving about proton in H-atom