I. What to recall about motion in a central potential
II. Example and solution of the radial equation for a particle trapped within radius “a”
III. The spherical square well

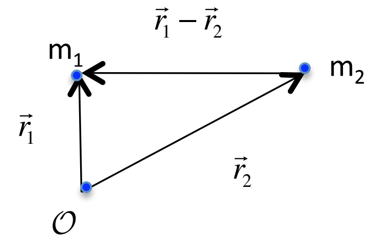
(Re-)Read Chapter 12 Section 12.3 and 12.4

I. What to recall about motion in a central potential

$V = V(|\vec{r}_1 - \vec{r}_2|)$ between masses m_1 and m_2

Recall the time-independent Schrodinger Equation:

$$H\Psi = E\Psi$$



$$\overbrace{\left[\frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(|\vec{r}_1 - \vec{r}_2|)\right]}^{H}\Psi = E\Psi$$

To convert this into a separable PDE, define

$$\frac{1}{M} = \frac{1}{m_1} + \frac{1}{m_2}$$

$$M = m_1 + m_2$$

$$R = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{M}$$

$$\vec{r} = \vec{r}_1 - \vec{r}_2$$

$$\vec{P} = \vec{p}_1 + \vec{p}_2$$

$$\frac{\vec{p}}{\mu} = \frac{\vec{p}_1}{m_1} - \frac{\vec{p}_2}{m_2}$$

Then you get

$$H = \underbrace{\frac{p^2}{2M}}_{\text{Ignore center of mass motion}} + \underbrace{\frac{p^2}{2\mu} + V(|\vec{r}|)}_{\text{Focus on this "}H_\mu\text{"}}$$

$$H_\mu = \frac{p^2}{2\mu} + V(r)$$

$$= \frac{-\hbar^2\nabla^2}{2\mu} + V(r)$$

In spherical coordinates:

$$\nabla^2 = \frac{1}{r^2}\left(r^2\frac{\partial}{\partial r}\right) + \underbrace{\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}}_{\frac{1}{r^2}\left(\frac{-L^2}{\hbar^2}\right)}$$

the angular momentum operator

Plug this ∇^2 into H_μ

Write out $\mathrm{H}_\mu \,|\Psi\rangle = E\,|\Psi\rangle$

Project into $\langle \mathrm{r},\theta,\varphi|$ space:

$$\left\{\frac{-\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{L^2}{\hbar^2 r^2}\right] + V(r)\right\}\langle r,\theta,\varphi\,|\,\Psi\rangle = E\langle r,\theta,\varphi\,|\,\Psi\rangle$$

Guess that $\langle \mathrm{r},\theta,\varphi\,|\,\Psi\rangle = R(r)f(\theta,\varphi)$

Separate the equation, the constant of separation turns out to be $\ell(\ell+1)$.

$\mathrm{f}(\theta,\varphi)$ turns out to be $\mathrm{Y}_\ell^m(\theta,\varphi)$

Then the R equation is:

$$\boxed{\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2\mu r^2}{\hbar^2}\big[V(r) - E\big] = \ell(\ell+1)}$$

"Form 1" of the radial equation

You can get an alternative completely equivalent form of this equation if you derive

$\mu \equiv \mathrm{rR}$

Then you get

$$\frac{-\hbar^2}{2\mu}\frac{d^2u}{dr^2}+\left[V+\frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right]u=Eu \qquad \text{"Form 2" of the radial equation}$$

*Choose either Form 1 or Form 2 depending upon what V is--

pick whichever gives and easier equation to solve

*Remember the boundary conditions on R:

$\mathrm{rR}(\mathrm{r}\to\infty)\to 0 \qquad \mathrm{BC1}$

$\mathrm{rR}(\mathrm{r}\to 0)\to 0 \qquad \mathrm{BC2}$

Procedure for finding the total $\Psi(\vec{\mathrm{r}},\mathrm{t})$ for a system in a central potential:

(i) Get V(r)

(ii) Plug it into the radial equation (either Form 1 or Form 2),

solve for R and the energies E_i

(iii) Multiply that R by $\mathrm{Y}_\ell^m(\theta,\varphi)$ and $\mathrm{e}^{-iE_it/\hbar}$ to get $\Psi(\mathrm{r,t})=\mathrm{RYe}^{-iE_it/\hbar}$

II. Example-Solution of the radial equation for a particle trapped within radius "a"

$$V=\begin{cases} 0 & \text{for } r < a \\ \infty & \text{for } r > a \end{cases}$$

This is also called a "spherical box"

Recall the radial equation in Form 1 (without the substitution u=rR):

$$\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)+\frac{2\mu}{\hbar^2}\left(E-V(r)-\frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right)\right]R=0$$

Since V=∞ for r > a, the wave function cannot have any portion beyond r > a.

So just solve the equation for r < a.

Plug in V=0 (r < a)

$$\left[\underbrace{\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)}+\underbrace{\frac{2\mu E}{\hbar^2}}-\frac{\ell(\ell+1)}{r^2}\right]R=0$$

expand this: call this "k^2"

$$\frac{1}{r^2}\left(r^2\frac{d^2}{dr^2}+2r\frac{d}{dr}\right)$$

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}+k^2-\frac{\ell(\ell+1)}{r^2}\right]R=0$$

Define $\rho \equiv kr$, so $\dfrac{1}{r} = \dfrac{k}{\rho}$

Then $\dfrac{d}{dr} = \dfrac{d\rho}{dr}\dfrac{d}{d\rho} = k\dfrac{d}{d\rho}$

$$\frac{d^2}{dr^2} = \frac{d}{dr}\left(k\frac{d}{d\rho}\right) = \frac{d\rho}{dr}\frac{d}{d\rho}\left(k\frac{d}{d\rho}\right) = k^2\frac{d^2}{d\rho^2}$$

Plug this in:

$$\left[k^2\frac{d^2}{d\rho^2} + \frac{2k^2}{\rho}\frac{d}{d\rho} + k^2 - \ell(\ell+1)\frac{k^2}{\rho^2}\right]R = 0$$

$$\left[\frac{d^2}{d\rho^2} + \frac{2}{\rho}\frac{d}{d\rho} + \left(1 - \frac{\ell(\ell+1)}{\rho^2}\right)\right]R = 0$$

Normalization not yet specified

The solution of this equation is $R(\rho) = \boxed{Cj_\ell(\rho)} + \boxed{Dn_\ell(\rho)}$

Spherical Neuman function,
Irregular @ r=0, so get D=0

$$j_\ell(\rho) \equiv \left(\frac{\pi}{2\rho}\right)^{1/2} \underbrace{J_{\ell+\frac{1}{2}}(\rho)}$$

"spherical Bessel function"

"ordinary Bessel function
of half-odd integer order"

examples: $j_0(\rho) = \dfrac{\sin\rho}{\rho}$

$$j_1(\rho) = \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho}$$

I. Particle in 3-D spherical well (continued)
II. Energies of a particle in a finite spherical well

Read Chapter 13

Now apply the BC: $\underbrace{\text{the wave function R must} = 0 \text{ @ } r = a}_{j_\ell(ka) = 0}$

whenever a Bessel function = 0 its argument (here: (ka)) is called a "zero" of the spherical Bessel function

and these columns are labelled by n

In spectroscopy the rows are labelled by:

			n=1	n=2	n=3	etc.
S	$j_{\ell=0}$	for ka =	3.14	6.28	9.42	...
P	$j_{\ell=1}$	for ka =	4.49	7.73	...	...
D	$j_{\ell=2}$	for ka =	5.76	9.10	...	...
F	$j_{\ell=3}$	...				
etc.						

Summarize:

$$\Psi^{\text{time-independent}}_{\substack{3-D \\ \text{central potential}}} = R \cdot Y_\ell^m$$

spherical harmonic

where $R = C \cdot j_\ell$

Because each j_ℓ has zeros at several n's,
we have to specify n too,
so $R \equiv R_{n\ell}$

Because $k^2 \equiv \dfrac{2\mu E}{\hbar^2}$, the boundary condition that $j_\ell(ka) = 0$ gives the allowed energies.

Recipe to find an allowed energy:

(i) Pick the n, ℓ levels that you want. (Example: pick n = 2, ℓ = 0)

(ii) Find the zero of that Bessel function $\left(ka\begin{pmatrix} n=2 \\ j_\ell = 0 \end{pmatrix} = 6.28 \right)$

(iii) Plug into $j_\ell(ka) = 0$

$$ka\begin{pmatrix} n=2 \\ j_\ell = 0 \end{pmatrix} = 6.28$$

$$\downarrow$$

$$k^2 a^2 = (6.28)^2$$

use $k^2 \equiv \dfrac{2\mu E}{\hbar^2}$

$$\downarrow$$

$$\frac{2\mu E_{\ell=0}^{n=2}}{\hbar^2} a^2 = (6.28)^2$$

$$\downarrow$$

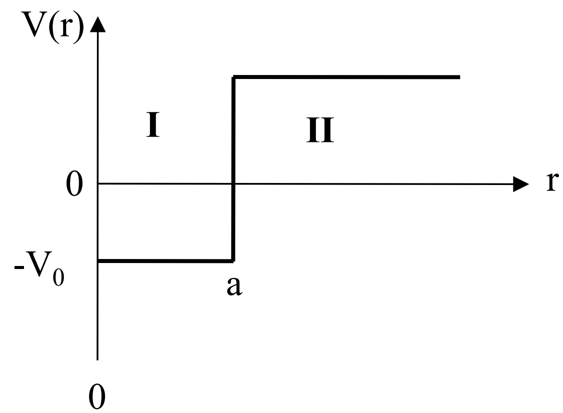
$$\boxed{E_{\ell=0}^{n=2} = \frac{(6.28)^2 \hbar^2}{2\mu a^2}}$$

I. Energies of a particle in a finite spherical square well

III. Energies of a particle in a finite spherical square well

Consider

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



This actuall looks very much like the potential between 2 nucleons in the nucleus

Solve this analogously to 1-D square well procedure

(i) Define regions I and II

(ii) Plug in V into radial equation in each region

Pick Form 2, so solve for u=rR

(iii) Apply BC @ $r = 0, a, \infty$

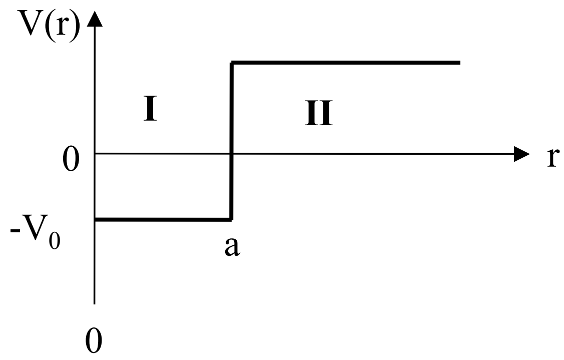
This leads to quantized E

(we'll stop here)

(iv) Normalize if you want the exact form of Ψ

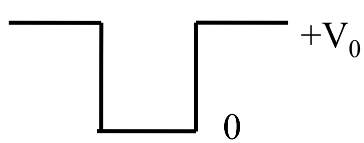
Carry out this procedure, first for $\ell = 0$ only, then for general ℓ:

Case I: Find allowed energies of a particle in an $\ell = 0$ state of a finite spherical square well



(i) define regions I and II

Notice that the particle in the well will have E < 0 just because of the way we defined the potential
*This is just a convention (i.e. a choice of the origin for the V scale), but since it is common we will use it.
Notice this is a different convention that the one we used for the 1-D square well

That was: 

but the *forms* of the solution inside and outside of the well (sinkx or e^{-kx}) are unaffected by the choice of origin.

Because E is intrinsically negative, we can write:

E = -|E| when we wish

Recall Form 2 of the radial equation:

$$\frac{-\hbar^2}{2\mu}\frac{d^2u}{dr^2}+\left[V+\frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right]u=Eu$$

when $\ell=0$ this is:

$$\frac{-\hbar^2}{2\mu}\frac{d^2u}{dr^2}+Vu=Eu$$

This is exactly the same form as for the 1-D square well, so the wavefunctions "in" will have the same form as the "$\Psi's$" for the 1-D square well

(ii) Plug in V:

Make a table as we did in Chapter 4:

	Region I	Region II
	$V = -V_0$	$V = 0$
General time-independent Radial equation:	$\left[\frac{-\hbar^2}{2\mu}\frac{d^2u}{dr^2}+V_0\right]u=Eu$	$\left[\frac{-\hbar^2}{2\mu}\frac{d^2u}{dr^2}\right]u=Eu$
Solve Radial equation to get:	"allowed region solution:" $u_I = A\sin k_1 r + B\cos k_1 r$	"forbidden region solution:" $u_{II} = Ce^{+k_2 r} + De^{-k_2 r}$
where:	$k_1 \equiv \frac{\sqrt{2\mu(V_0+E)}}{\hbar} = \frac{\sqrt{2\mu(V_0-\mid E\mid)}}{\hbar}$	$k_2 \equiv \frac{\sqrt{2\mu(-E)}}{\hbar} = \frac{\sqrt{2\mu\mid E\mid}}{\hbar}$

(iii) Apply BC's:

BC1: $rR(r \to \infty) \to 0$

$u(r \to 0) \to 0$ So B=0

BC2: $rR(r \to \infty) \to 0$

$u(r \to \infty) \to 0$ So C=0

BC3: $u_I(r{=}a) = u_{II}(r{=}a)$

$A\sin k_1 a = De^{-k_2 a}$ "equation 1"

BC4: $\frac{du_I}{dr}(r{=}a) = \frac{du_{II}}{dr}(r{=}a)$

$k_1 A\cos k_1 a = -k_2 De^{-k_2 a}$ "equation 2"

Divide $\text{equation 1} \big/ \text{equation 2}$:

$k_1 \cot k_1 a = -k_2$ This has the same form (variation in some factors or 2) as the Class 2 (or odd) solutions to the 1-D square well.

Multiply both side by a:

$k_1 a \cot k_1 a = -k_2 a$

$-\cot k_1 a = \frac{k_2 a}{k_1 a}$

$\downarrow$

Define $\lambda \equiv \dfrac{2\mu V_0 a^2}{\hbar^2}$

Define y $\equiv$ $k_1 a = \dfrac{a\sqrt{2\mu(V_0 - |E|)}}{\hbar}$

Notice that

$$k_2 a = \frac{a\sqrt{2\mu|E|}}{\hbar} = \sqrt{\frac{(2\mu V_0 a^2) - [2\mu(V_0 - |E|)a^2]}{\hbar^2}}$$

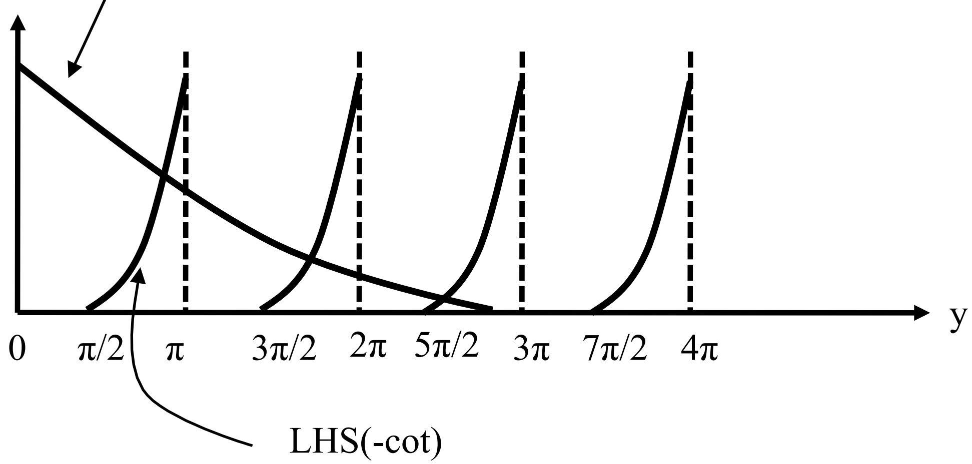
$$= \sqrt{\lambda - y^2}$$

$$-\cot y = \frac{\sqrt{\lambda - y^2}}{y}$$

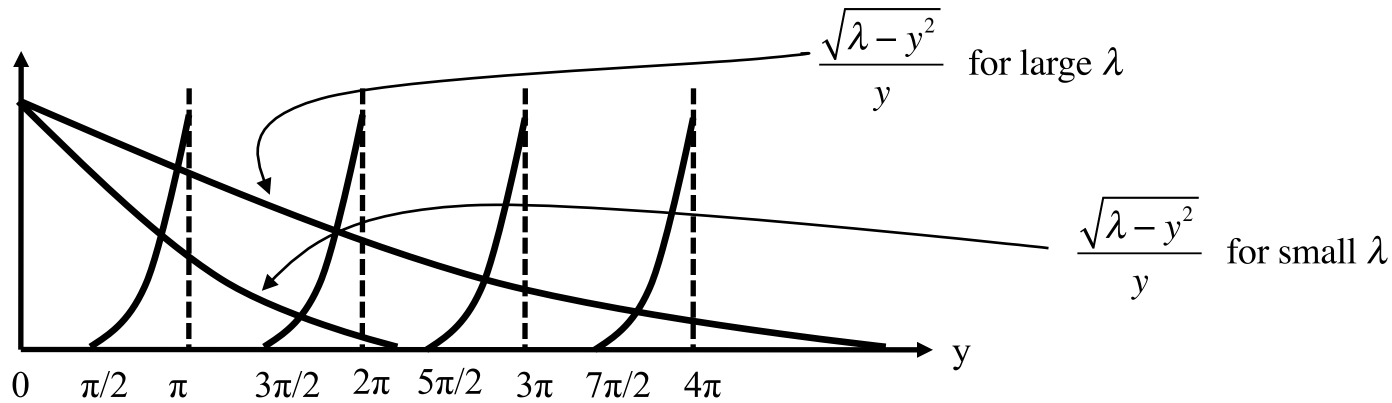
Plot both sides versus y.

Intersection points are solution to the equation:

(use the identity that -cotx = +tan($\dfrac{\pi}{2}$+x))



How the value of λ affects the plot:



*Notice if λ is very small there may be NO interactions

proportional to $V_0 a^2$

well depth (well width)^2

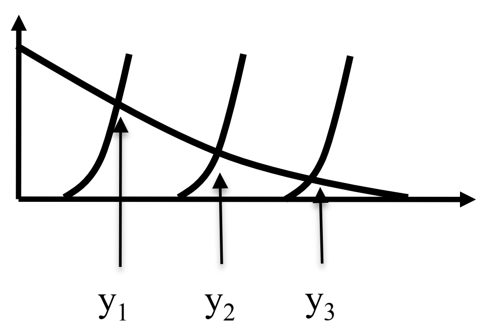
To find E:

Locate graphically, or computationally, the y-coordinates of the points where:

$$-\cot y = \frac{\sqrt{\lambda - y^2}}{y}$$

Call these y_i

Example:



Then plug in the definition of y:

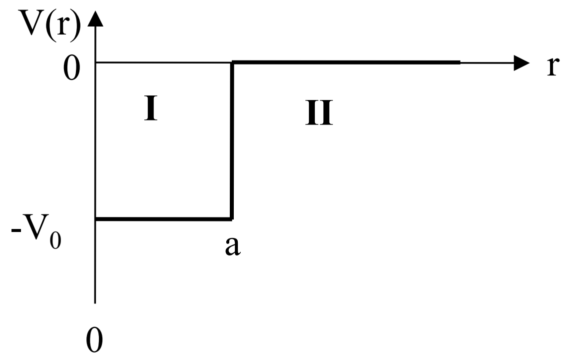
$$y_i = \frac{a}{\hbar}\sqrt{2\mu(V_0 - |E_i|)}$$

Plug in these values of a, u, V_0, $\hbar$, to solve for E_i

Alternatively if you measure the E_i (for example the bound state energies of a deuteron), you can work backwards to find $V_0 a^2$.

Recall Case 1 was for $\ell = 0$ only. Now,

Case 2: Find the allowed energies for finite spherical square well for a particle in an arbitrary ℓ state.



(i) Regions I II

(ii) In this case Form 1 of the Radial equation is easier to solve:

$$\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)+\frac{2\mu}{\hbar^2}\left(E-V(r)-\frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right)\right]R=0$$

expand the derivative and write E = -|E|

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}+\frac{2\mu}{\hbar^2}\left(-|E|-V(r)-\frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right)\right]R=0$$

Make Table:

	Region I	Region II
	V = -V_0	V = 0
General time-independent Radial equation:	$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}+\frac{2\mu}{\hbar^2}\left(V_0-\lvert E\rvert-\frac{\ell(\ell+1)}{r^2}\right)\right]R=0$	$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{2\mu\lvert E\rvert}{\hbar^2}-\frac{\ell(\ell+1)}{r^2}\right]R=0$
To solve this define:	$k_{\mathrm{I}}\equiv\frac{\sqrt{2\mu(V_0-\lvert E\rvert)}}{\hbar}$	$k_{\mathrm{II}}\equiv\frac{\sqrt{2\mu\lvert E\rvert}}{\hbar}$
and	$\rho_{\mathrm{I}}\equiv k_{\mathrm{I}}r$ (just like p.6 in notes)	$\rho_{\mathrm{II}}\equiv ik_{\mathrm{II}}r$
Then the radial equation becomes:	$\left[\frac{d^2}{d\rho_{\mathrm{I}}^2}+\frac{2}{\rho_{\mathrm{I}}}\frac{d}{d\rho_{\mathrm{I}}}+\left(1-\frac{\ell(\ell+1)}{\rho_{\mathrm{I}}^2}\right)\right]R=0$	$\downarrow$
The solution is:	$R_\ell^{\mathrm{I}}(\rho_{\mathrm{I}})=A_\ell j_\ell(\rho_{\mathrm{I}})+B_\ell j_\ell(\rho_{\mathrm{I}})$	

I. Energies of a particle in a finite spherical square well, continued
II. The Hydrogen Atom

If $\rho_{\mathrm{II}} \equiv ik_{\mathrm{II}} r$

Then $\dfrac{1}{r} = \dfrac{ik_{\mathrm{II}}}{\rho_{\mathrm{II}}}$

$$\frac{d}{dr} = \frac{d\rho_{\mathrm{II}}}{dr}\frac{d}{d\rho_{\mathrm{II}}} = ik_{\mathrm{II}}\frac{d}{d\rho_{\mathrm{II}}}$$

$$\frac{d^2}{dr^2} = \frac{d}{dr}\left(ik_{\mathrm{II}}\frac{d}{d\rho_{\mathrm{II}}}\right) = \frac{d\rho_{\mathrm{II}}}{dr}\frac{d}{d\rho_{\mathrm{II}}}\left(ik_{\mathrm{II}}\frac{d}{d\rho_{\mathrm{II}}}\right) = ik_{\mathrm{II}}ik_{\mathrm{II}}\frac{d^2}{d\rho_{\mathrm{II}}^2} = -k_{\mathrm{II}}^2\frac{d^2}{d\rho_{\mathrm{II}}^2}$$

Plug these in: then the Radial Equation becomes

$$\left[-k_{\mathrm{II}}^2\frac{d^2}{d\rho_{\mathrm{II}}^2} + \frac{2ik_{\mathrm{II}}}{\rho_{\mathrm{II}}}ik_{\mathrm{II}}\frac{d}{d\rho_{\mathrm{II}}} - k_{\mathrm{II}}^2 + \frac{\ell(\ell+1)k_{\mathrm{II}}^2}{\rho_{\mathrm{II}}^2}\right]R = 0$$

Multiply through by (-1):

$$\left[\frac{d^2}{d\rho_{\mathrm{II}}^2} + \frac{2}{\rho_{\mathrm{II}}}\frac{d}{d\rho_{\mathrm{II}}} + 1 - \frac{\ell(\ell+1)}{\rho_{\mathrm{II}}^2}\right]R = 0$$

Again the solution is $\underline{\mathrm{R}_\ell^{\mathrm{II}}(\rho_{\mathrm{II}}) = C_\ell \mathrm{j}_\ell(\rho_{\mathrm{II}}) + D_\ell \mathrm{n}_\ell(\rho_{\mathrm{II}})}$

Since Region II does not include r=0, we do no thave to discard the Neumann for n_ℓ.

Since we have not yet fixed C and D, we can rewrite $\mathrm{R}_\ell^{\mathrm{II}}$ as a different form of linear combination of j_ℓ and n_ℓ.

In particular we could define

$\mathrm{h}_\ell^{(1)} \equiv \mathrm{j}_\ell + i\mathrm{n}_\ell$ and

$\mathrm{h}_\ell^{(2)} \equiv \mathrm{j}_\ell - i\mathrm{n}_\ell$ "The spherical Hankel functions"

Then

$$\underline{\mathrm{R}_\ell^{\mathrm{II}}(\rho_{\mathrm{II}}) = C'_\ell h_\ell^{(1)}(\rho_{\mathrm{II}}) + D'_\ell h_\ell^{(2)}(\rho_{\mathrm{II}})}$$

(iii) Now apply the boundary conditions:

BC1: $\mathrm{rR}(\mathrm{r} \to 0) \to 0$ This is satisfied by $\mathrm{R}_\ell^{\mathrm{I}} = Aj_\ell(\rho_{\mathrm{I}}) = Aj_\ell(k_{\mathrm{I}}r)$

BC2: $\mathrm{rR}(\mathrm{r} \to \infty) \to 0$

Examine the $\mathrm{h}_\ell(\mathrm{r} \to \infty)$:

$$\mathrm{j}_\ell(\rho \to \infty) \to \frac{1}{\rho}\cos\left[\rho - \frac{(\ell+1)\pi}{2}\right]$$

$$\mathrm{n}_\ell \equiv (-1)^{\ell+1}\left(\frac{\pi}{2\rho}\right)^{1/2} J_{-\ell-\frac{1}{2}}(\rho)$$

$$\xrightarrow[\rho\to\infty]{} \frac{1}{\rho}\sin\left[\rho - \frac{(\ell+1)\pi}{2}\right]$$

Plug these in:

I. Energies of a particle in a finite spherical square well (continued)
II. The Hydrogen Atom

$$h_\ell^{(1)}(\rho_{\mathrm{II}}) \xrightarrow[r\to\infty]{} \frac{1}{ik_{\mathrm{II}}r}\cos\left[ik_{\mathrm{II}}r - \frac{(\ell+1)\pi}{2}\right] + i\frac{1}{ik_{\mathrm{II}}r}\sin\left[ik_{\mathrm{II}}r - \frac{(\ell+1)\pi}{2}\right]$$

$$= \frac{1}{ik_{\mathrm{II}}r}\left\{\cos\left[ik_{\mathrm{II}}r - \frac{(\ell+1)\pi}{2}\right] + i\sin\left[ik_{\mathrm{II}}r - \frac{(\ell+1)\pi}{2}\right]\right\}$$

Ignore the phases for now

Recall $\mathrm{e}^{i\theta} = \cos\theta + i\sin\theta$

Here "θ" is $ik_{\mathrm{II}}r$

$$\sim \frac{1}{ik_{\mathrm{II}}r}\left\{e^{i(ik_{\mathrm{II}}r)}\right\}$$

$$\sim \frac{1}{ik_{\mathrm{II}}r}\left\{e^{-k_{\mathrm{II}}r}\right\}$$ This $\to 0$ as r $\to \infty$ so it satisfies the BC

$$h_\ell^{(2)}(\rho_{\mathrm{II}}) \xrightarrow[r\to\infty]{} \frac{1}{ik_{\mathrm{II}}r}\cos\left[ik_{\mathrm{II}}r - \frac{(\ell+1)\pi}{2}\right] - i\frac{1}{ik_{\mathrm{II}}r}\sin\left[ik_{\mathrm{II}}r - \frac{(\ell+1)\pi}{2}\right]$$

$$\sim \frac{1}{ik_{\mathrm{II}}r}\left\{e^{+k_{\mathrm{II}}r}\right\}$$ This blows up as r $\to \infty$ so we must set its coefficient D′=0

BC3: $\mathrm{R}^{\mathrm{I}}(r=a) = \mathrm{R}^{\mathrm{II}}(r=a)$

$$\underline{\mathrm{A}\mathrm{j}_\ell(k_{\mathrm{I}}a) = C' h_\ell^{(1)}(k_{\mathrm{II}}a)}$$

BC4: $\dfrac{\partial \mathrm{R}^{\mathrm{I}}}{\partial r}(r=a) = \dfrac{\partial \mathrm{R}^{\mathrm{II}}}{\partial r}(r=a)$

$$\underline{\mathrm{A}\frac{d}{dr}\mathrm{j}_\ell(k_{\mathrm{I}}a) = C'\frac{d}{dr}h_\ell^{(1)}(k_{\mathrm{II}}a)}$$

Divide $\dfrac{\text{BC4}}{\text{BC3}}$ to eliminate the normal Bat. coefficients:

$$\frac{\frac{d}{dr}j_\ell(k_\text{I}a)}{j_\ell(k_\text{I}a)} = \frac{\frac{d}{dr}h_\ell^{(1)}(k_\text{II}a)}{h_\ell^{(1)}(k_\text{II}a)}$$

For a specific V_0, a, u, and ℓ, one can solve this for the bound states E_i

I. The Hydrogen Atom

What this means is "the eigen functions and eigen energies possible for the electron in a one-electron atom"

energy levels

This is just the central potential problem again, now for

$$V = \frac{-Ze^2}{r}$$

\# protons in nucleus

Charge of electron

So we know that Ψ_electron will have the form $\Psi \sim R(r)Y_\ell^m$

because of this (ℓ, m), also subscript the Ψ':Ψ_ℓ^m

So the most general Ψ must be a linear combination of all possible Ψ_ℓ^m's, so

$$\Psi = \sum_{\ell,m}\Psi_\ell^m = \sum_{\ell,m}R(r)Y_\ell^m(\theta,\varphi)$$

The Y_ℓ^m's are standard functions so we can ignore them for now. We will find R and then just multiply by Y_ℓ^m later.

To find R, recall the Radial Equation (Form 2):

$$\frac{-\hbar^2}{2\mu}\frac{d^2u}{dr^2}+\left[V+\frac{\hbar^2\ell(\ell+1)}{2\mu r^2}\right]u=Eu \qquad \text{(where } u \equiv rR\text{)}$$

Consider bound states, so se E=-|E|

Defined as E<0

Plug in $V=\dfrac{-Ze^2}{r}$

$$\left[\frac{-\hbar^2}{2\mu}\frac{d^2u}{dr^2}+\frac{\hbar^2\ell(\ell+1)}{2\mu r^2}-\frac{Ze^2}{r}+|E|\right]u=Eu$$

To simplify the form of the equation, multiply through by $\dfrac{-2\mu}{\hbar^2}$ and define

$$\rho \equiv \left(\frac{8\mu|E|}{\hbar^2}\right)^{\frac{1}{2}} r$$

So

$$\frac{1}{r}=\left(\frac{8\mu|E|}{\hbar^2}\right)^{\frac{1}{2}}\frac{1}{\rho}$$

and

$$\frac{d}{dr}=\frac{d\rho}{dr}\frac{d}{d\rho}=\left(\frac{8\mu|E|}{\hbar^2}\right)^{\frac{1}{2}}\frac{d}{d\rho}$$

and

$$\frac{d^2}{dr^2} = \frac{d}{dr}\left[\left(\frac{8\mu\,|E|}{\hbar^2}\right)^{\frac{1}{2}}\frac{d}{d\rho}\right]$$

$$= \frac{d\rho}{dr}\frac{d}{d\rho}\left[\left(\frac{8\mu\,|E|}{\hbar^2}\right)^{\frac{1}{2}}\frac{d}{d\rho}\right]$$

$$= \left(\frac{8\mu\,|E|}{\hbar^2}\right)^{\frac{1}{2}}\frac{d^2}{d\rho^2}$$

Plug these in:

$$\left[\left(\frac{8\mu\,|E|}{\hbar^2}\right)\frac{d^2}{d\rho^2} - \frac{\ell(\ell+1)}{\rho^2}\left(\frac{8\mu\,|E|}{\hbar^2}\right) + \frac{2\mu}{\hbar^2}\frac{Ze^2}{\rho}\left(\frac{8\mu\,|E|}{\hbar^2}\right)^{\frac{1}{2}} - \frac{2\mu\,|E|}{\hbar^2}\right]u = 0$$

divide through by $\left(\frac{8\mu\,|E|}{\hbar^2}\right)$:

$$\left[\frac{d^2}{d\rho^2} - \frac{\ell(\ell+1)}{\rho^2} + \boxed{\frac{\frac{2\mu Ze^2}{\hbar^2}}{\left(\frac{8\mu\,|E|}{\hbar^2}\right)^{\frac{1}{2}}}}\frac{1}{\rho} - \frac{1}{4}\right]u = 0$$

$$\downarrow$$

$$\boxed{\frac{Ze^2}{\hbar}\sqrt{\frac{\mu}{2\,|E|}}}$$

call this "λ"

$$\left[\frac{d^2}{d\rho^2} - \frac{\ell(\ell+1)}{\rho^2} + \left(\frac{\lambda}{\rho} - \frac{1}{4}\right)\right]u = 0$$

Procedure to solve: this is similar to the one for the analytic (non-a^+a) solution of the harmonic oscillator.

Recall the 2 radial BC's: BC1: $u(r \to \infty) \to 0$; BC2: $u(r \to 0) \to 0$.

(i) consider the case where $\rho \to \infty$

This eliminates the $\frac{1}{\rho}, \frac{1}{\rho^2}$ terms:

Then the equation is approximately:

$$\frac{d^2u}{d\rho^2} - \frac{u}{4} = 0 \qquad \text{(for } u(\rho \to \infty) \text{ only)}$$

$$\Big\downarrow \text{ solution}$$

$$u \sim Ae^{\frac{-\rho}{2}} + Be^{\frac{+\rho}{2}}$$

Apply BC1:
Recall a physically acceptable Ψ
(or u) must $\to 0$ for $r \to \infty, \rho \to \infty$
so B must $= 0$.

(ii) Consider the case where $\rho \to 0$

Then the $\frac{1}{\rho^2}$ term dominates the $\frac{1}{\rho}$ and the $\frac{1}{4}$ terms, so the equation is approximately:

$$\left[\frac{d^2}{d\rho^2} - \frac{\ell(\ell+1)}{\rho^2}\right]u = 0$$

$$\Big\downarrow \text{ solution}$$

$$u = C\rho^{-\ell} + D\rho^{\ell+1}$$

I. The Hydrogen Atom (continued)
II. Facts about the principal quantum number n
III. The wavefunction of an e^- in hydrogen

Apply BC2: u($\rho \to 0$) $\to 0$, so
C=0

(iii) Now insist that the exact solution of the equation have a form which will join up with these asymptotic cases smoothly.

Assume u(all ρ) = $e^{\left(\frac{-\rho}{2}\right)}\rho^{\ell+1}H(\rho)$

H(ρ)=$\sum_i a_i \rho^i$

H $\neq$ a hamiltonian here

Plug this into the full equation:

$$\left[\frac{d^2}{d\rho^2} - \frac{\ell(\ell+1)}{\rho^2} + \left(\frac{\lambda}{\rho} - \frac{1}{4}\right)\right] e^{\left(\frac{-\rho}{2}\right)}\rho^{\ell+1}H(\rho) = 0$$

$$\frac{d}{d\rho}\left\{ e^{\left(\frac{-\rho}{2}\right)}\left[\rho^{\ell+1}\frac{dH}{d\rho} + (\ell+1)\rho^{\ell}H\right] - \frac{1}{2}e^{\left(\frac{-\rho}{2}\right)}\rho^{\ell+1}H(\rho)\right\}$$

$$\frac{d}{d\rho}\left\{ e^{\left(\frac{-\rho}{2}\right)}\rho^{\ell+1}\frac{dH}{d\rho} + e^{\left(\frac{-\rho}{2}\right)}(\ell+1)\rho^{\ell}H - e^{\left(\frac{-\rho}{2}\right)}\rho^{\ell+1}\frac{H}{2}\right\}$$

$$= e^{\left(\frac{-\rho}{2}\right)}\left[\rho^{\ell+1}\frac{d^2H}{d\rho^2} + (\ell+1)\rho^{\ell}\frac{dH}{d\rho}\right] - \frac{1}{2}e^{\left(\frac{-\rho}{2}\right)}\rho^{\ell+1}\frac{dH}{d\rho}$$

$$+ (\ell+1)e^{\left(\frac{-\rho}{2}\right)}\left[\ell\rho^{\ell-1}H + \rho^{\ell}\frac{dH}{d\rho}\right] - \frac{1}{2}e^{\left(\frac{-\rho}{2}\right)}(\ell+1)\rho^{\ell}H$$

$$- \frac{1}{2}e^{\left(\frac{-\rho}{2}\right)}\left[(\ell+1)\rho^{\ell}H + \rho^{\ell+1}\frac{dH}{d\rho}\right] + \frac{1}{4}e^{\left(\frac{-\rho}{2}\right)}\rho^{\ell+1}H$$

and divide out $e^{\left(\frac{-\rho}{2}\right)}$:

$$[\rho^{\ell+1}\frac{d^2H}{d\rho^2}+(\ell+1)\rho^{\ell}\frac{dH}{d\rho}-\frac{1}{2}\rho^{\ell+1}\frac{dH}{d\rho}$$
$$+(\ell+1)\ell\rho^{\ell-1}H+(\ell+1)\rho^{\ell}\frac{dH}{d\rho}-\frac{1}{2}(\ell+1)\rho^{\ell}H$$
$$-\ \frac{1}{2}(\ell+1)\rho^{\ell}H-\frac{1}{2}\rho^{\ell+1}\frac{dH}{d\rho}+\frac{1}{4}\rho^{\ell+1}H-\ell(\ell+1)\rho^{\ell-1}H+\lambda\rho^{\ell}H-\frac{1}{4}\rho^{\ell+1}H]\ =0$$

Collect terms:

$$\rho^{\ell+1}\frac{d^2H}{d\rho^2}+\left[(\ell+1)\rho^{\ell}-\frac{1}{2}\rho^{\ell+1}+(\ell+1)\rho^{\ell}-\frac{1}{2}\rho^{\ell+1}\right]\frac{dH}{d\rho}$$
$$+\left[(\ell+1)\ell\rho^{\ell-1}-\frac{1}{2}(\ell+1)\rho^{\ell}-\frac{1}{2}(\ell+1)\rho^{\ell}+\frac{1}{4}\rho^{\ell+1}-\ell(\ell+1)\rho^{\ell-1}+\lambda\rho^{\ell}-\frac{1}{4}\rho^{\ell+1}\right]H=0$$

Collect terms:

$$\rho^{\ell+1}\frac{d^2H}{d\rho^2}+\left[2(\ell+1)\rho^{\ell}-\rho^{\ell+1}\right]\frac{dH}{d\rho}$$
$$+\left[-(\ell+1)\rho^{\ell}+\lambda\rho^{\ell}\right]H=0$$

Divide through by ρ^{ℓ} :

$$\rho\frac{d^2H}{d\rho^2}+\left[2\ell+2-\rho\right]\frac{dH}{d\rho}-\left[\ell+1-\lambda\right]H=0$$

*Notice that for a given value of ℓ, this is an eigenvalue equation for H with eigenvalue = λ.

Recall H here is part of a wavefunction and not a hamiltonian

Plug in H=$\sum a_i \rho^i$

$$\frac{dH}{d\rho}=\sum i a_i \rho^{i-1}$$

$$\frac{d^2H}{d\rho^2}=\sum i(i-1) a_i \rho^{i-2}$$

$$\rho\sum i(i-1)a_i\rho^{i-2} + (2\ell + 2 - \rho)\sum i a_i \rho^{i-1} - (\ell + 1 - \lambda)\sum a_i \rho^i = 0$$

$$\sum i(i-1)a_i\rho^{i-1} + (2\ell+2)\sum i a_i \rho^{i-1} - \sum(\ell + 1 - \lambda + i) a_i \rho^i = 0$$

$$\sum i(i-1+2\ell+2)a_i\rho^{i-1} - \sum(\ell + 1 - \lambda + i) a_i \rho^i = 0$$

$$\sum i(i+2\ell+1)a_i\rho^{i-1} - \sum(\ell + 1 - \lambda + i) a_i \rho^i = 0$$

Set coefficients of each power of ρ separately = 0:

Set coefficients of each power of ρ separately = 0:

ρ^0 $\quad 1(2\ell+2)a_1 - (\ell + 1 - \lambda + 0)a_0 = 0$

ρ^1 $\quad 2(2\ell+2)a_2 - (\ell + 1 - \lambda + 1)a_1 = 0$

ρ^2 $\quad 3(2\ell+4)a_3 - (\ell + 1 - \lambda + 2)a_2 = 0$

ρ^3 $\quad 4(2\ell+5)a_4 - (\ell + 1 - \lambda + 3)a_3 = 0$

ρ^4 $\quad 5(2\ell+6)a_5 - (\ell + 1 - \lambda + 4)a_4 = 0$

ρ^n $\quad (n+1)(2\ell + n+2)a_{n+1} - (\ell + 1 - \lambda + n)a_n = 0$

$$a_{n+1} = \frac{\left[(\ell+1+n) - \lambda\right]}{(n+1)(2\ell+n+2)} a_n$$ Recursive realtion for the a_i

This relationship between the a_i is like the one for an exponential function.
To see this compare:

The "H(ρ)" series

$$\frac{a_{n+1}}{a_n} = \frac{\ell+1+n-\lambda}{(n+1)(2\ell+n+2)}$$

when n $\rightarrow$ large

$$\approx \frac{n}{n \cdot n} \sim \frac{1}{n}$$

"The e^ρ series", $e^\rho = \sum \frac{\rho_i}{i}$, so $a_i = \frac{1}{i!}$

$$\frac{a_{n+1}}{a_n} = \frac{\frac{1}{(n+1)!}}{\frac{1}{n!}} = \frac{n!}{(n+1)!} = \frac{1}{n+1}$$

when n $\rightarrow$ large

$$\sim \frac{1}{n}$$

So if H(ρ) is not truncated, what we have so far is

$$\begin{aligned} u(\rho) &= e^{\frac{-\rho}{2}}\rho^{\ell+1}H(\rho) \\ &= e^{\frac{-\rho}{2}}\rho^{\ell+1}e^{+\rho} \\ &= e^{\frac{+\rho}{2}}\rho^{\ell+1} \xrightarrow[\rho\to\infty]{} \infty \end{aligned}$$

To force u to be a physically acceptable wavefunction, truncate the series H

Pick $\underbrace{\text{some i}}_{\text{call it } i_{max}}$ whose a_i is the highest non-zero a_i

Recall $a_{i+1} = \dfrac{[\ell+1+i-\lambda]}{(i+1)(2\ell+i+2)}a_i$

when $i=i_{max}$

$a_i = a_{i\,max}$

$a_{i+1} = 0$

$0 = \ell+1+i_{max} - \lambda$

$\lambda=\ell+1+i_{max}$

Since i and ℓ and 1 are all integers,

λ must be an integer.

Rename it "n"

I. Facts about the principal quantum number n (continued)
II. The wavefunction of an e^- in hydrogen
III. Probability current for an e^- in hydrogen

Facts about λ=n

1. "n" is called the Principal Quantum Number

2. Recall the definition

$$n=\lambda=\frac{Ze^2}{\hbar}\sqrt{\frac{\mu}{2|E_n|}},\ \text{so}$$

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

These are the allowed bound state energies of the Coulomb potential.

3. $n=\ell+i_{max}+1$, so

$n \geq \ell+1 \quad (i_{max}=0,1,...)$

$\ell \leq n-1$, or $\ell_{max}=n-1$

4. Notice no matter how large n is, its E_n will always be slightly <0, so at lease weakly bound.

So this potential $V=\frac{-Ze^2}{r}$ has an infinite number of bound energy states (unlike the square well).

5. Energy degeneracies:

(i) due to $\ell \rightarrow$ The energy depends only on n, but for each n, there are $\underbrace{\text{n possible values of } \ell}_{\ell=0,\,1,...,\,n-1}$

(ii) due to m $\rightarrow$ For each ℓ, m can be $-\ell, -\ell+1, ..., 0, ..., \ell-1, \ell$

(iii) total due to m and ℓ is then

$$\sum_{\ell=0}^{n-1}(\underbrace{2\ell+1}_{\text{number m values}})=n^2$$

(this ignores spin for now)

6. A (2ℓ+1)-fold degeneracy of m-values is characteristic of a spherically symmertric potential.

II. The wavefunction of an e^- in hydrogen

Recall we found that

$$\Psi^{\text{time-independent}}_{\substack{\text{e in}\\ \text{hydrogen}}} = \boxed{R} \cdot Y_\ell^m$$

to solve the R equation we used Form 2,

so we defined $\rho = \sqrt{\frac{8\mu|E|}{\hbar^2}} r = 2\sqrt{\frac{2\mu|E|}{\hbar^2}} r = 2kr$

and u=rR

$$R = \frac{1}{r}u = \frac{1}{r}\left[e^{\frac{-\rho}{2}}\rho^{\ell+1}\boxed{H(\rho)}\right]$$

$$\sum_i^{i_{\max}} a_i \rho^i$$

$$= \frac{2k}{\rho}\left[e^{\frac{-\rho}{2}}\rho^{\ell+1}H(\rho)\right]$$

$$= e^{\frac{-\rho}{2}}\rho^{\ell}2k\boxed{\sum_i^{i_{\max}} a_i \rho^i}$$

These turn out to be famous functions

the associated Lguerre Polynomials, $L_q^P(\rho)$

$$H(\rho)=\underbrace{-L_{n+\ell}^{2\ell+1}(\rho)}$$

$$L_q^P(x)=\frac{d^P}{dx^P}\underbrace{L_q(x)}$$

$$L_q(x)\equiv e^x\frac{d^q}{dx^q}(x^q e^{-x})$$

Example of L_q's and L_q^P's:

$L_0(x)=1$ $\qquad$ $L_1'(x)=-1$

$L_1(x)=1-x$ $\qquad$ $L_2'(x)=-4+2x$

$L_2(x)=2-4x+x^2$ $\qquad$ $L_3'(x)=2$

Summary:

$$R(\rho)=Ce^{\frac{-\rho}{2}}\rho^{\ell}\left(-L_{n+\ell}^{2\ell+1}(\rho)\right)$$

Normalization not determined yet

Normalize:

$$1=\int|\Psi|^2 dV_0L=\underbrace{\int|Y_\ell^m|^2\,d\Omega}\underbrace{\int|R|^2\,r^2\,dr}$$

automatically=1
because the Y's
are normalized

$$\int |R(\rho)|^2\, r^2\, dr$$

$$\downarrow \qquad \text{recall } \rho\text{=2kr, so } r^2 dr = \frac{1}{(2k)^3}\rho^2 d\rho$$

$$\frac{C^2}{(2k)^3}\underbrace{\int \left[L_{n+\ell}^{2\ell+1}(\rho)\right]^2 e^{-\rho}\rho^{2\ell}\rho^2 d\rho}_{\frac{2n\left[(n+\ell)!\right]^3}{(n-\ell-1)!}}$$

So $C = \left\{\dfrac{(2k)^3(n-\ell-1)!}{2n\left[(n+\ell)!\right]^3}\right\}^{\frac{1}{2}}$

Plug in:

$$\boxed{R = -\left\{\frac{(2k)^3(n-\ell-1)!}{2n\left[(n+\ell)!\right]^3}\right\}^{\frac{1}{2}} \rho^{\ell} e^{\frac{-\rho}{2}} L_{n+\ell}^{2\ell+1}(\rho) \qquad \text{where } \rho = 2kr = \sqrt{\frac{8\mu|E|}{\hbar^2}}\, r}$$

*It is common to derive $a_0 \equiv \dfrac{-\hbar^2}{\mu e^2}$, the Bohr radius.

Then $\rho = \sqrt{\dfrac{8\mu|E|}{\hbar^2}}\, r$ can be simplified:

$$\downarrow \qquad \text{Recall } E = \frac{-Z^2 e^4 \mu}{\hbar^2 2n^2}, \text{ so } |E| = \frac{Z^2 e^4 \mu}{\hbar^2 2n^2}$$

$$\rho = \sqrt{\frac{8\mu}{\hbar^2}\frac{Z^2 e^4 \mu}{\hbar^2 2n^2}}\, r$$

$$\downarrow$$

I. Facts about $\Psi_{e \text{ in hydrogen}}$
II. Probability current for an e^- in hydrogen

Read 2 handouts
Read Chapter 14

$$\rho = \frac{2\mu Z e^2 r}{\hbar^2 n} = \frac{2Zr}{a_0 n}$$

Specific $R_{n\ell}(r)$'s are listed in Goswami Eq. 13.23

In general, $\boxed{R_{n\ell}(r) = \left\{ \left(\frac{2Z}{na_0} \right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3} \right\}^{\frac{1}{2}} \left(\frac{2Zr}{a_0 n} \right)^{\ell} e^{\frac{-Zr}{a_0 n}} L_{n+\ell}^{2\ell+1}\left(\frac{2Zr}{a_0 n} \right)}$

Facts about the $\Psi_{e \text{ in hydrogen}}$:

(i) They are totally orthogonal:

$$\int \Psi_{n'\ell'm'} \Psi_{n\ell m}\, dVolume = \delta_{n'n}\ \delta_{\ell'\ell}\ \delta_{m'm}$$

due to the $e^{im\varphi}$ in the Y_ℓ^m

due to the orthogonality of Legendre Polynomials P_ℓ

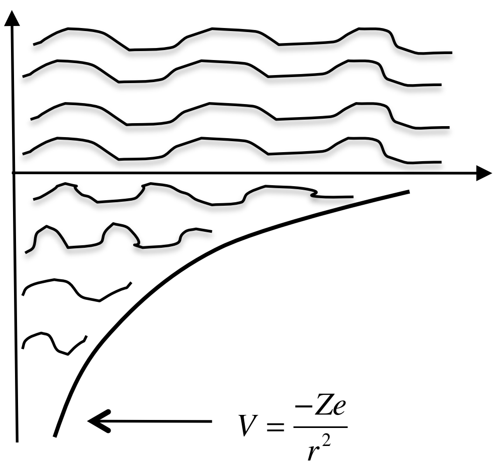
recall Y_ℓ^m =(Normalization constant) $\cdot\, e^{im\varphi} \cdot P_\ell^m$

The Laguerre Polynomials are orthogonal in n

(ii) Recall what a complete set of ℓ' functions is: $\underbrace{\text{it can act as a } \textit{basis} \text{ for its space}}$

i.e., any possible wavefunction in that space can be written as a linear combination of the elements of the basis.

The comlete set of eigen functions of the hydrogen atom look like:



E>0 (scattering) states
(we will study these in Chapter 23)

E<0 (bound) states

So the bound states do not form a complete set by themselves

(iii) Notice all the $R_{n\ell} \sim r^{\ell}$

So for $\ell > 0$, $R_{n\ell}(r=0) = 0$

No probability of finding the e^- at the origin in these states

for $\ell = 0$, $R_{n\ell}(r=0) = \text{constant}$

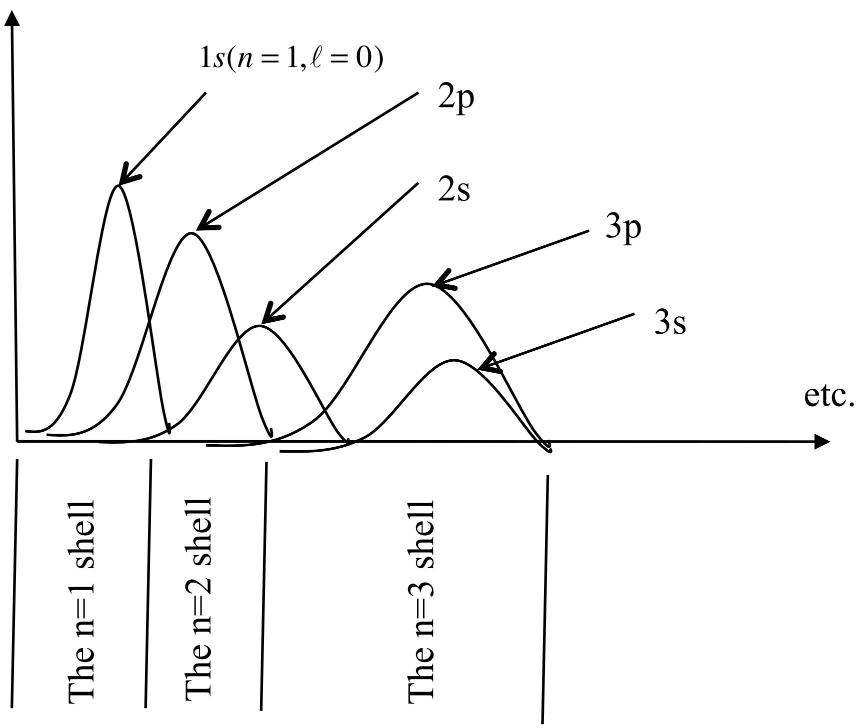
So the ground state e^- has a spherical probability distribution which includes the origin. So the ground state e^- has finite probability to be found *inside* the nucleus.

(iv) To calculate the probability of finding the e^- at a specific r, calculate

Probability(r)=$r^2 \, |R_{n\ell}|^2$

This is similar to $P(x)=|\Psi(x)|^2$. The r^2 adjusts to spherical coordinates.

When you calculate $r^2 \,|\, R \,|^2$ you find



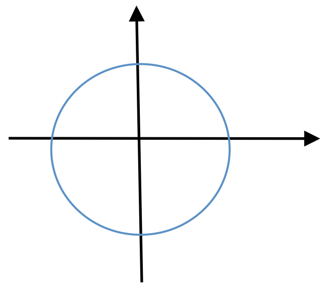
(v) to calculate the probability of finding the e^- at a particular θ,

calculate Probability(θ)=$|Y_\ell^m(\theta,\varphi)|^2 \sin\theta d\theta d\varphi$

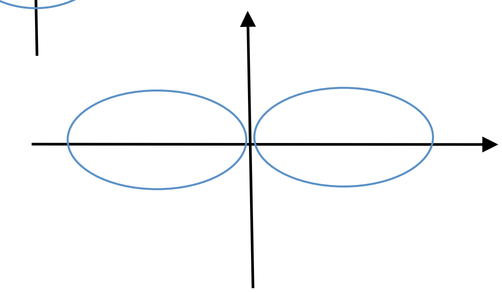
since the φ appears in $e^{im\varphi}$ it
will disappear from the probability

You find:

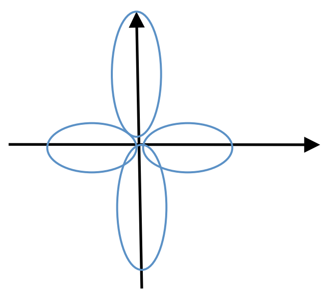
Prob(ℓ=0,m=0) = s-orbital



Prob(ℓ=1) = p-orbital



Prob(ℓ=2) = d-orbital



etc.

(vi) Recall Parity Ps the operation that inverts the Ψ through the origin

So $P\Psi(r,\theta,\varphi)=R(r)(-1)^{\ell}Y_{\ell}^{m}(\pi-\theta,\pi+\varphi)$

unchanged by P

So $\boxed{P(\Psi_{\text{e in hydrogen}}) = (-1)^{\ell}\Psi}$

Review Syllabus
Read Goswami section 13.3 and chapter 14 plus the preceding chapter as necessary for reference

Read Chapter 14

I. Probability current for an e^- in hydrogen
II. The effect of an EM field on the eigen functions and eigen values of a charged particle
III. The Hamiltonian for the combined system of a charged particle in a general EM field

I. Probability current for an e^- in Hydrogen

Recall the definition of probability current:

$$\vec{J}=\frac{\hbar}{2\mu i}\left(\Psi^*\vec{\nabla}\Psi-\Psi\vec{\nabla}\Psi^*\right)$$

Recall this describes the spatial flow of probability

$\rightarrow$ NOT necessarily the motion of the point of maximum probability

$\rightarrow$ definitely not the motion of a particle whose probability of location is related to Ψ

Calculate J for the e^- in Hydrogen:

Plug in $\Psi_{n\ell m}=R_{n\ell}(r)\cdot\underbrace{Y_\ell^m(\theta,\varphi)}_{\text{call this } \Theta(\theta)\cdot e^{im\varphi}}\cdot e^{-iE_nt/\hbar}$

call this $\Theta(\theta)\cdot e^{im\varphi}$, where $\Theta(\theta)$ is pure real

and $\vec{\nabla}_{\substack{\text{spherical}\\ \text{coordinates}}}=\hat{r}\frac{\partial}{\partial r}+\hat{\theta}\frac{1}{r}\frac{\partial}{\partial\theta}+\hat{\varphi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}$

you get:

$$J=\frac{\hbar}{2\mu i}\left[\left(R^*\theta^*e^{-im\varphi}e^{iEt/\hbar}\right)\nabla\left(R\theta e^{im\varphi}e^{-iEt/\hbar}\right)-\left(R\theta e^{im\varphi}e^{-iEt/\hbar}\right)\nabla\left(R^*\theta^*e^{-im\varphi}e^{iEt/\hbar}\right)\right]$$

Notice since $R^*=R$

and $\theta^*=\theta$,

that $R^*\theta^*\nabla R\theta-R\theta\nabla R^*\theta^*=0$

so consider only the φ part of the equation

$$\text{So } \vec{J} = \hat{\varphi}\frac{\hbar}{2\mu i}\left[\left(R^*\theta^*\mathrm{e}^{-im\varphi}e^{iEt/\hbar}\right)\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\left(R\theta\mathrm{e}^{im\varphi}e^{-iEt/\hbar}\right) - \left(R\theta\mathrm{e}^{im\varphi}e^{-iEt/\hbar}\right)\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\left(R^*\theta^*\mathrm{e}^{-im\varphi}e^{iEt/\hbar}\right)\right]$$

$$= \hat{\varphi}\frac{\hbar}{2\mu i}R^2\theta^2\left(\mathrm{e}^{-im\varphi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\mathrm{e}^{im\varphi} - \mathrm{e}^{im\varphi}\frac{1}{r\sin\theta}\frac{\partial}{\partial\varphi}\mathrm{e}^{-im\varphi}\right)$$

$$= \hat{\varphi}\frac{\hbar R^2\theta^2}{2\mu i}\left(\mathrm{e}^{-im\varphi}\frac{1}{r\sin\theta}im\mathrm{e}^{im\varphi} - \mathrm{e}^{im\varphi}\frac{1}{r\sin\theta}(-im)\mathrm{e}^{-im\varphi}\right)$$

$$= \hat{\varphi}\frac{\hbar R^2\theta^2 m}{\mu r\sin\theta}$$

$$\boxed{= \hat{\varphi}\frac{|\Psi|^2\, m\hbar}{\mu r\sin\theta}}$$

Note this current is

(i) time-independent

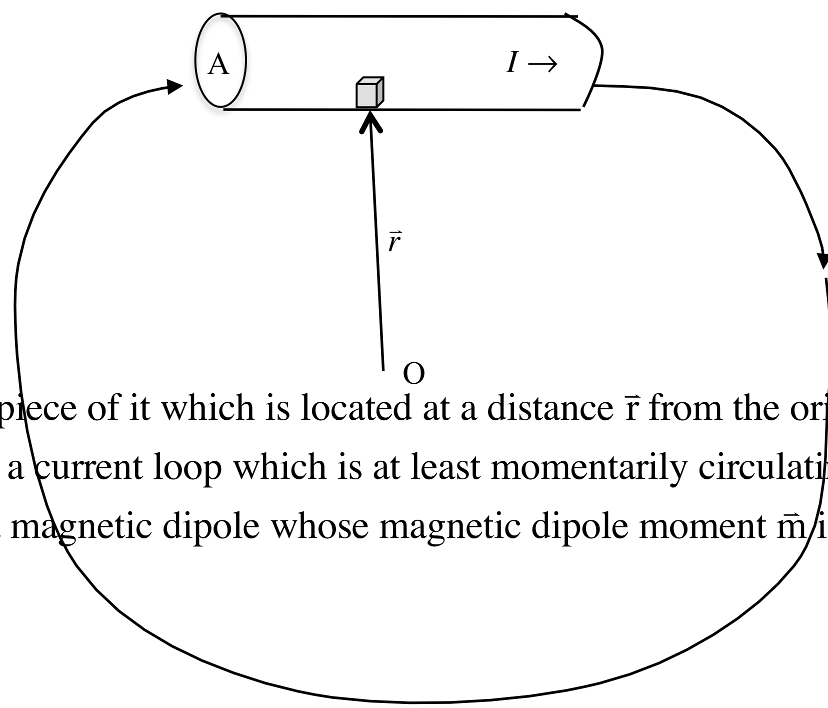
(ii) circulating around the z-axis (not $\hat{\varphi}$) but remaining symmetric about it

(iii) NOT the same as an orbiting e^-

This circulating $\vec{J}$ is related to the magnetic dipole moment of the e^-

To show this recall from EM:

If you have a physical charged current density $\vec{J}_e = \dfrac{\vec{I}}{A}$



Consider a differentially small piece of it which is located at a distance $\vec{r}$ from the origin.

This piece forms an element of a current loop which is at least momentarily circulating relative to the origin.

This is physically identical to a magnetic dipole whose magnetic dipole moment $\vec{m}$ is given by:

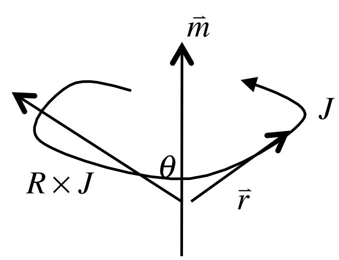
$$\vec{m} \equiv \frac{1}{2} \int_{\substack{\text{volume}\\ \text{where } J_e \\ \text{circulates}}} \vec{r} \times \vec{J}_e(\vec{r})\, dVolume$$

we can convert our probability current $\vec{J}$ into a physical charged current $\vec{J}_e$ by multiplying by the charge:

$$\vec{J}_e = \left(\frac{-e}{c}\right)\vec{J}$$

Then the magnetic dipole moment of the e^- is given by

$$\vec{m} \equiv \frac{1}{2} \int_{\text{volume}} \vec{r} \times \left(\frac{-e}{c}\right)\vec{J}\, dVolume$$



Notice since $\vec{J}=|J|\hat{\varphi}$, $\vec{m}$ must be $|\vec{m}|\hat{z}$

So we only need $\left(\vec{r} \times \vec{J}\right)_z = rJ\sin\theta$

So we want

$$m=m_z=\frac{-e}{2c}\int rJ\sin\theta\, dVolume$$

$$=\frac{-e}{2c}\int\frac{r\,|\Psi|^2\; m\hbar}{\mu r\sin\theta}\sin\theta\, dVolume$$

$$=\frac{-em\hbar}{2\mu c}\int|\Psi|^2\; dVolume$$

by normalization

$$\text{so } m_z=\boxed{\frac{-e\hbar}{2\mu c}}\cdot m$$

quantum number "m"

This factor is called the Bohr magneton

Magnitude of the z-component of magnetic dipole moment of the e^-

Since $m\hbar$ is the eigen value of L_z, m must be the eigen value of some operator "$\frac{-e}{2\mu c}L_z$"

call this the z component m_z magnetic moment operator M

Then $\boxed{M=\frac{-e}{2\mu c}L}$

angular momentum operator

magnetic momentum operator

I. The effect of an EM field on the eigen functions and eigen values of a charged particle
II. The Hamiltonian for the combined system of a charged particle in a general EM field
III. The Hamiltonian for a charged particle in a uniform, static B field

Read Chapter 15

The effect of and EM field on the eigen functions and eigen values of a charged particle

General plan:

(i) We know the Hamiltonian of a free particle of momentum, $\vec{\mathrm{p}}$:

$$\mathrm{H}=\frac{p^2}{2\mu}$$

(ii) Find the H for that same particle with charge q in an EM field $(\vec{\mathrm{E}},\vec{\mathrm{B}})$

we will find that $\mathrm{H}\sim\frac{p^2}{2\mu}+[\mathrm{stuff}]\cdot\mathrm{B}+[\mathrm{stuff}']\mathrm{B}^2$

we will study each kind separately

II. The Hamiltonian for the combined system of a charged particle in a general EM field

Procede to find H:

(i) Recall that *classically*, $\mathrm{H}\equiv\sum_{i=1}^{3}p_i\dot{x}_i-\mathcal{L}$

where the $\begin{cases} x_i = \text{canonical coordinates} \\ p_i = \text{canonical momenta} \end{cases}$

(ii) Find L. Recall that equations of motion must be obtainable from it via

$$\frac{\partial L}{\partial x_i}-\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_i}\right)=0$$

I. The Hamiltonian for a charged particle in an EM field
II. The Hamiltonian for a charged particle in a uniform, static B field
III. The normal Zeeman effect

(iii) Plug in $\mathcal{L}$ to get H, then convert everything possible to operators

Carry this out:

To find $\mathcal{L}$, recall that usually

$\mathcal{L}$=T-V

Here T=$\frac{1}{2}\mu v^2$ (use μ for mass everywhere)

What is v? Recall the EM field has 2 kinds of potential:

scalar potential φ and vector potential $\vec{\mathrm{A}}$

How to combine them? (we can't just say "V=φ+$\vec{\mathrm{A}}$")

It turns out the $\mathcal{L}$=$\frac{1}{2}\mu v^2 - q\varphi + \frac{q}{c}\vec{A}\cdot\vec{V}$

To demonstrate this, we will show that

$$\frac{\partial L}{\partial x_i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_i}\right) = 0 \quad \text{(Lagrange's equation)}$$

successfully produces the known Lorentz Force Law $\vec{\mathrm{F}}$=q$\vec{\mathrm{E}}$+$\frac{q\vec{v}}{c}\times\vec{B}$

To plug into this, we need:

$$\frac{\partial L}{\partial x_i} = -q\frac{\partial\varphi}{\partial x_i} + \frac{q}{c}\vec{v}\bullet\frac{\partial A}{\partial x_i}$$

To find $\frac{\partial L}{\partial x_i}$, notice we can expand:

$$\mathcal{L}=\frac{1}{2}\mu\sum \dot{x}_i^2 - q\varphi + \frac{q}{c}\sum A_i\dot{x}_i$$

So $\dfrac{\partial L}{\partial \dot{x}_i} = \mu\dot{x}_i + \dfrac{q}{c}A_i$ [Note this is the definition of the canonical momentum p_i]

Then $\dfrac{d}{dt}\left(\dfrac{\partial L}{\partial \dot{x}_i}\right) = \mu\ddot{x}_i + \dfrac{q}{c}\dfrac{d}{dt}A_i$

$$\frac{\partial A}{\partial t} + \sum_j \frac{\partial x_j}{\partial t}\frac{\partial A}{\partial x_j}$$

$$\frac{\partial A}{\partial t} + \vec{v}\cdot\nabla\vec{A}_i$$

Plug all this into Lagrange's Equation:

$$\text{-q}\frac{\partial \varphi}{\partial x_i} + q\frac{\vec{v}}{c}\frac{\partial \vec{A}}{\partial x_i} = \mu\ddot{x}_i + \frac{q}{c}\left(\frac{\partial A_i}{\partial t} + \vec{v}\cdot\nabla\vec{A}_i\right)$$

Reorder:

$$\mu\ddot{x}_i = \text{-q}\frac{\partial \varphi}{\partial x_i} - \frac{q}{c}\frac{\partial A_i}{\partial t} + \frac{q\vec{v}}{c}\frac{\partial \vec{A}}{\partial x_i} - \frac{q}{c}\vec{v}\cdot\nabla\vec{A}_i$$

This equation concerns component i (i=1, 2, or 3)

of a vector equation. Generalize to the full vector equation.

$$\mu\vec{a}(=\vec{F})=\text{q}\underbrace{\left(-\nabla\varphi - \frac{1}{c}\frac{\partial A}{\partial t}\right)}_{\vec{E}} + \frac{q}{c}\underbrace{\left[\vec{\nabla}(\vec{v}\cdot\vec{A}) - (\vec{v}\cdot\nabla)\vec{A}\right]}_{}$$

To understand this recall:

$$\text{So } \frac{q}{c}\left[\nabla(\vec{v}\cdot A) - (v\cdot\nabla)A\right]$$

$$u\times(y\times z) = y(u\cdot z) - z(u\cdot y)$$

Plug in v ∇ $\vec{A}$

$$=\nabla(\vec{v}\cdot A) - (v\cdot\nabla)A$$

$$\frac{q}{c}\left[v\times(\nabla\times A)\right]$$

So we have $\vec{F} = q\vec{E} + \frac{q}{c}\vec{v}\times\vec{B}$

So we know we have the right Lagrangian

Now find $H = \sum p_i\dot{x}_i - L$

$$= \sum \underbrace{\left(\mu\dot{x}_i + \frac{q}{c}A_i\right)}_{\text{canonical momentum}}\dot{x}_i - \left(\frac{1}{2}\mu\sum\dot{x}_i^2 - q\varphi + \frac{q}{c}\sum A_i\dot{x}_i\right)$$

$$= \sum\frac{\mu}{2}\dot{x}_i^2 + q\varphi$$

$$= \sum_i \frac{\left(\mu\dot{x}_i\right)^2}{2\mu} + q\varphi$$

Now use again the definition of canonical momenta

$$p_i = \mu\dot{x}_i + \frac{q}{c}A_i$$

$$\sum\left(\mu\dot{x}_i\right)^2 = \sum\left(p_i - \frac{q}{c}A_i\right)^2$$

$$\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2$$

$$\boxed{H=\frac{\left(\vec{p}-\frac{q\vec{A}}{c}\right)^2}{2\mu}+q\varphi}$$

By convention,	if the particle is:	then we use:
	an e^- (negative)	q=-e
	e^+ (positive)	q=+e

II. The Hamiltonian for a charged particle in a *uniform* static $\vec{B}$ field

Recall general $H=\frac{1}{2\mu}\left(\vec{p}-\frac{q\vec{A}}{c}\right)^2+q\varphi$

$$=\frac{1}{2\mu}\left(\vec{p}^2-\frac{q}{c}\underbrace{\left(\vec{A}\cdot\vec{p}+\vec{p}\cdot\vec{A}\right)}_{\text{we want to simplify this}}+\frac{q^2}{c^2}\vec{A}^2\right)+q\varphi$$

Recall:

$[f(x),p]=i\hbar\frac{\partial f}{\partial x}$ (see next page)

Generalize to 3D: $[\vec{f}(\vec{r}),p]=i\hbar\vec{\nabla}\cdot\vec{f}$

Plug in A, then:

$[A,p]=i\hbar\vec{\nabla}\cdot\vec{A}$

now recall that for a *static* $\vec{B}$ field, $\vec{\nabla}\cdot\vec{A}=0$

Show this:

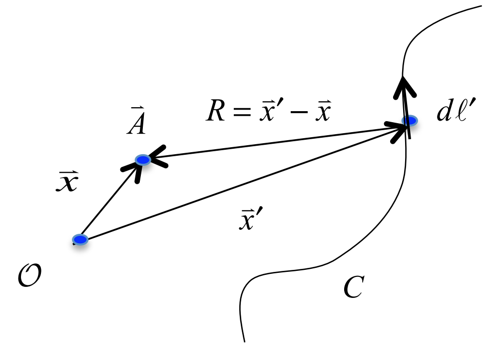
Recall in general B can be produced by (i) a uniform current and (ii) a $\frac{\partial E}{\partial t}$.

Consider the *static* case, so A=f(I) only

Recall if a current $\vec{I}$ flows along a segment $d\ell'$ of path C, then the vector potential $\vec{A}$ at distance R from C is

$$\vec{A}(x) = \frac{\mu_0}{4\pi}\frac{I d\ell'}{R}$$

this is permiability, not mass



$$\vec{A}_{\substack{\text{due to}\\ \text{total C}}}(x) = \frac{\mu_0}{4\pi}\oint_C \frac{I d\vec{\ell}'}{R}$$

$$\nabla = \frac{\partial}{\partial x} \text{ etc. not } \frac{\partial}{\partial x'}$$

$$\vec{\nabla}\cdot\vec{A} = \vec{\nabla}\left[\frac{\mu_0}{4\pi}\oint_C \frac{I d\vec{\ell}'}{R}\right] = \frac{\mu_0 I}{4\pi}\oint_C \vec{\nabla}\frac{d\vec{\ell}'}{R}$$

Recall $\nabla\cdot\left(u\vec{V}\right) = \vec{V}\cdot\nabla u + u\left(\vec{\nabla}\cdot\vec{V}\right)$

$\frac{1}{R}$ $\quad d\vec{\ell}'$

$$d\vec{\ell}'\cdot\vec{\nabla}\left(\frac{1}{R}\right) + \frac{1}{R}\vec{\nabla}d\vec{\ell}'$$

0 since ∇ operating on unprimed coordinates only, and $d\vec{\ell}'$ is constructed of primed coordinates

$$\vec{\nabla}\left(\frac{1}{R}\right) = \vec{\nabla}\left(\frac{1}{\sqrt{\sum (x_i' - x_i)}}\right) = -\vec{\nabla}\left(\frac{1}{R}\right)$$

Rewrite:

$$\vec{\nabla}\cdot\vec{A} = \frac{-\mu_0 I}{4\pi}\oint_C \vec{\nabla}'\left(\frac{1}{R}\right)d\vec{\ell}'$$

Recall Stoke's Theorem:

for any vector $\vec{v}$,

$$\oint_C \vec{v}\, d\vec{\ell} = \int_{\substack{\text{surface enclosed}\\ \text{by C}}} \left(\vec{\nabla}\times\vec{v}\right) dArea$$

I. The Hamiltonian for an e^- in a uniform, static B field (continued)

II. The normal Zeeman effect

III. Response to the e^- to the B^2 term

IV. Summary of e^- response to static uniform $B\hat{z}$

V. The discovery of spin

$$\vec{\nabla}\cdot\vec{A} = \frac{-\mu_0 I}{4\pi}\int_S \left[\nabla' \times \left(\nabla'\left(\frac{1}{R}\right)\right)\right]\cdot d\,\text{Area}$$

but the curl of a divergence always = 0

So, $\vec{\nabla}\cdot\vec{A} = 0$ for static B

Return to $\left[A, p\right] = i\hbar\underbrace{\vec{\nabla}\cdot\vec{A}}_{0}$

So $\vec{\text{A}}$ and $\vec{\text{p}}$ commute.

So $(\vec{\text{A}}\cdot\vec{\text{p}}+\vec{\text{p}}\cdot\vec{\text{A}})=2\vec{\text{A}}\cdot\vec{\text{p}}$

Then $\text{H}_{\text{e in static B}} = \dfrac{1}{2\mu}\left[p^2 - \dfrac{q}{c}2\vec{A}\cdot\vec{\text{p}} + \dfrac{q^2}{c^2}A^2\right] + q\varphi$

Now further restrict this *static* (no time dependence) B field to be also *uniform*:

call it $\vec{\text{B}}=|\text{B}|\hat{\text{z}}$

constant, 1 directional, no position dependence

In general for any B,

$\vec{B} = \vec{\nabla}\times\vec{A}$

$$\overbrace{B_x\hat{x} + B_y\hat{y} + B_z\hat{z}} = \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}\right)\hat{x} + +\left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}\right)\hat{y} + \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)\hat{z}$$

When $\vec{\text{B}}=|\text{B}|\hat{\text{z}}$, this reduces to:

$$0 + 0 + \text{B}\hat{\text{z}} = 0 + 0 + \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right)\hat{z}$$

There is more than 1 solution to this. One is:

$$\begin{pmatrix} A_x = -\dfrac{1}{2} B \cdot y \\ A_y = \dfrac{1}{2} B \cdot x \\ A_x = 0 \end{pmatrix}$$

This can be written precisely as:

$$\vec{\mathrm{A}} = \frac{1}{2} \vec{B} \times \vec{r}$$

Plug this into $\vec{\mathrm{A}} \cdot \vec{\mathrm{p}}$:

$$\frac{1}{2}\left(\vec{B} \times \vec{r}\right) \cdot \vec{\mathrm{p}}$$

$$\Big\downarrow$$

Recall the vector identity:

$\vec{\mathrm{u}} \cdot (\vec{\mathrm{y}} \cdot \vec{z}) = (\vec{u} \cdot \vec{y}) \cdot \vec{z}$

$$\frac{1}{2} \vec{B} \cdot \underbrace{\left(\vec{r} \times \vec{\mathrm{p}}\right)}$$

$\vec{\mathrm{L}}$= angular momentum

Now we have:

$$\mathrm{H}_{\text{e in static B}} = \frac{1}{2\mu}\left[p^2 - \frac{q}{c} \cancel{2} \frac{1}{\cancel{2}} \vec{B} \cdot \vec{L} + \frac{q^2}{c^2} A^2 \right] + q\varphi$$

Plug in $\mathrm{A}^2 = \left[\frac{1}{2}\left(\vec{B} \times \vec{r}\right) \right]^2$

Recall $\vec{\mathrm{B}} \times \vec{\mathrm{r}} = \mathrm{Brsin}\theta$ and $\vec{\mathrm{B}} \cdot \vec{\mathrm{r}} = \mathrm{Brcos}\theta$

So

$$\left(\vec{\mathrm{B}} \times \vec{\mathrm{r}}\right)^2 = \mathrm{B}^2\mathrm{r}^2\mathrm{sin}^2\theta = B^2 r^2 (1 - \cos^2\theta) = B^2 r^2 - \left(\vec{\mathrm{B}} \cdot \vec{\mathrm{r}}\right)^2$$

So

$$\mathrm{A}^2 = \frac{1}{4}\left[B^2 r^2 - \left(\vec{\mathrm{B}} \cdot \vec{\mathrm{r}}\right)^2\right]$$

Plug this into H

$$\mathrm{H}_{\text{e in uniform static B}} = \frac{p^2}{2\mu} - \underbrace{\frac{q}{2\mu c}\vec{B} \cdot \vec{L}} + \frac{q^2}{8\mu c^2}\left(B^2 r^2 - \left(\vec{\mathrm{B}} \cdot \vec{\mathrm{r}}\right)^2\right) + q\varphi$$

note $\frac{q\vec{L}}{2\mu c}$ is the magnetic moment $\vec{\mathrm{M}}$ of the particle

Since we choose the coordinate system so that $\vec{\mathrm{B}} = \mathrm{B}\hat{\mathrm{z}}$,

$$\vec{B} \cdot \vec{L} = BL_z$$

and $\mathrm{r}^2 B^2 - \left(\vec{\mathrm{r}} \cdot \vec{\mathrm{B}}\right)^2 = (x^2 + y^2 + z^2)B^2 - (x^2 B_x^2 + y^2 B_y^2 + z^2 B_z^2) = (x^2 + y^2)B^2$

Then

$$\mathrm{H}_{\text{e in uniform static B}} = \frac{p^2}{2\mu} - \frac{q}{2\mu c}BL_z + \frac{q^2}{8\mu c^2}\left(B^2(x^2 + y^2)\right) + q\varphi$$

For an electron, q=-e, so

$$\boxed{\mathrm{H}_{\text{e in uniform static B}} = \frac{p^2}{2\mu} - \frac{eBL_z}{2\mu c} + \frac{e^2 B^2}{8\mu c^2}(x^2 + y^2) - e\varphi}$$

"μ" is the reduced mass of the system

*If you want the answer in mks units, set c=1

I. The normal Zeeman effect

II. Response to the e^- to the B^2 term

III. Summary of e^- response to static uniform $B\hat{z}$

IV. The discovery of spin

We will study the effect of each term separately upon the e's wavefunction and energy.

II. The Normal Zeeman Effect

Recall $H_{\text{e in uniform static B in } \hat{z}} = \dfrac{p^2}{2\mu} + \dfrac{eL_zB}{2\mu c} + \dfrac{e^2B^2(x^2+y^2)}{8\mu c^2} - e\varphi$

$= "H_0" + "H_1" + "H_2" \qquad -e\varphi$

compare relative sizes of H_1 and H_2

$$\frac{H_2}{H_1} = \frac{\dfrac{e^2B^2(x^2+y^2)}{8\mu c^2}}{\dfrac{eL_zB}{2\mu c}} = \frac{eB(x^2+y^2)}{4cL_z}$$

Plug in e = $1.6\text{x}10^{-19}$ C

B = 1 tesla = 10^4 gauss

$(x^2+y^2) \sim (5x10^{-11})^2$ m^2 (Bohr radius)^2

c = 1 (unitless) to convert Gaussian $\rightarrow$ MKS units

$L_z \sim m\hbar \sim \hbar = 1\text{x}10^{-34}$ Joule-seconds

Then,

$$\frac{H_2}{H_1} \sim \frac{(1.6\text{x}10^{-19})(1\text{ tesla})(5x10^{-11})^2\text{m}^2}{4(1)(1\text{x}10^{-34}J-\text{sec})} = 10^{-6}$$

So $H_2 \ll H_1$ for B<$10^5 - 10^6 T$

magnetic field at earth's surface is ~$0.5\text{x}10^{-4}$ T

superconducting magnets ~ 10 T

So, in a normal situation:

$$\mathrm{H}_{\text{e in uniform static B in }\hat{z}} \approx \frac{p^2}{2\mu} + \frac{eL_z B}{2\mu c} - e\varphi$$

Suppose $\varphi = \frac{ze}{r}$, so

$-e\varphi = \frac{-ze^2}{r}$

Then the e is in $\underbrace{\text{the Coulomb Field of its own nucleus}}_{\text{This gives it } \boxed{\mathrm{E}_n = \frac{-\mu z^2 e^4}{2\hbar^2 n^2}}}$

plus the extra $\vec{\mathrm{B}}$ field

Recall each energy level "n" is degenerate,

all of its ℓ and m levels have the same energy

How does this H_1 affect the e's energy levels?

$$\mathrm{H}_1\Psi_{n\ell m} = \frac{eL_z B}{2\mu c}\Psi_{n\ell m} = \underbrace{\left(\frac{eB}{2\mu c}\right)}\underbrace{L_z\Psi_{n\ell m}}_{m\hbar\Psi_{n\ell m}}$$

quantum number "m" NOT mass

call this collection

of constants "ω_L",

the Larmor frequency

So the presence of H_1 means that the different "m" levels are no longer degenerate; each has its own energy given by:

$$E_m = \frac{-\mu z^2 e^4}{2\hbar^2 n^2} + \omega_L m\hbar$$

So	without B	with B		
E		———	$\dfrac{-\mu z^2 e^4}{2\hbar^2 n^2} + \omega_L \hbar$	m=+1
↑	———	———	$\dfrac{-\mu z^2 e^4}{2\hbar^2 n^2}$	m=0
E of all levels		———	$\dfrac{-\mu z^2 e^4}{2\hbar^2 n^2} - \omega_L \hbar$	m=-1
with same n		———		m=-2
				etc.

The fact that a magnetic field can cause the levels designated by "m" change energy causes "m" to be called "The magnetic quantum number"

II. Response of the e- to the ~B^2 term

Recall $H = \dfrac{p^2}{2\mu} + \dfrac{eBL_z}{2\mu c} + \dfrac{e^2B^2(x^2+y^2)}{8\mu c^2} - e\varphi$

$$= \frac{p_z^2}{2\mu} + \frac{eBL_z}{2\mu c} + \underbrace{\frac{p_x^2+p_y^2}{2\mu} + \frac{e^2B^2(x^2+y^2)}{8\mu c^2}} \underbrace{- e\varphi}_{\text{ignore for now (let } \to 0)}$$

this is identical to the Harmonic Oscillator:

$$H_{\substack{2D\\ \text{Ho}}} = \frac{p_x^2}{2\mu} + \frac{p_y^2}{2\mu} + \frac{1}{2}k_1x^2 + \frac{1}{2}k_2y^2 \qquad \text{where } k_1 = k_2 = \frac{e^2B^2}{4\mu c^2}$$

From Chapter 9 (2-D systems)

$$\underset{\text{HO}}{\mathrm{H}_{2D}}\Psi = (n_x + n_y + 1)\hbar\omega\Psi$$

$$\omega = \sqrt{\frac{k}{\mu}} = \frac{eB}{2c\sqrt{\mu}}\frac{1}{\sqrt{\mu}} = \frac{eB}{2c\mu} = \omega_{\text{Larmor}}$$

III. Summary of e response to static uniform $B\hat{z}$

So far we found that

$$\mathrm{H} = \frac{p_z^2}{2\mu} + \frac{eBL_z}{2\mu c} + \underbrace{\frac{p_x^2 + p_y^2}{2\mu} + \frac{e^2B^2(x^2+y^2)}{8\mu c^2}}_{\mathrm{H}_{2D,\,HO}} - \underbrace{e\varphi}_{\text{Set} = 0 \text{ for now}}$$

Recall: a particular Ψ is simultaneously an e function of 2 operators $\vec{\mathrm{Y}}$ and $\vec{\mathrm{Z}}$ only if $[\vec{\mathrm{Y}},\hat{\mathrm{Z}}]=0$.

Notice $[\mathrm{p}_z, L_z] = 0$ since $\mathrm{L}_z = xp_y - yp_x$

$$[\mathrm{p}_z, \underset{\text{HO}}{H_{2\mathrm{D}}}] = 0$$

$$[L_z, \underset{\text{HO}}{H_{2\mathrm{D}}}] = 0$$

So all the terms of H have the $\underbrace{\text{same e function}}_{\text{call it "}\Psi_{nmk}\text{"}}$

Plug it in:

I. The Discovery of Spin

II. Filtering particles with a Stern-Gerlach apparatus

III. Experiments with filtered atoms

$$\mathrm{H}\Psi_{nmk} = \frac{p_z^2}{2\mu}\Psi_{nmk} + \frac{eBL_z}{2\mu c}\Psi_{nmk} + H_{\substack{2D\\HO}}\Psi_{nmk}$$

Recall: $\mathrm{p}_z\Psi = \hbar k\Psi$

$\mathrm{L}_z\Psi = m\hbar\Psi$

$H_{\substack{2D\\HO}}\Psi = (n_x + n_y + 1)\hbar\omega_L\Psi$

$$\mathrm{H}\Psi_{nmk} = \underbrace{\left[\frac{\hbar^2 k^2}{2\mu} + m\hbar\omega_L + (n_x + n_y + 1)\hbar\omega_L\right]}\Psi_{nmk}$$

But in general $\mathrm{H}\Psi = E\Psi$, so this must be "E"

$$\boxed{\mathrm{E}_{nmk} = \frac{\hbar^2 k^2}{2\mu} + (m + n_x + n_y + 1)\hbar\omega_L}$$

III. The discovery of spin

Suppose you wanted to measure the $\underbrace{\text{total angular momentum}}_{\text{call it } \vec{\mathrm{J}} \text{ as in Ch. 11 (Note: this J is not a current)}}$ of a particle

We showed in Chapter 13 that angular momentum $\propto$ magnetic moment

$$\frac{-e\vec{L}}{2\mu c} = \vec{\mathrm{M}}$$

Now call this "$\vec{\mathrm{J}}$" to be general, i.e. to allow for more than just orbital angular momentum

So $\vec{J} = \frac{-2\mu c\vec{M}}{e}$

So we want to design an apparatus to measure $\vec{M}$

Recall from E&M that if a magnetic dipole $\vec{M}$ is in a magnetic field $\vec{B}$ it feels a force on it which depends on the relative orientation of $\vec{M}$ and $\vec{B}$:

$\vec{F} = \vec{\nabla}(\vec{M} \cdot \vec{B})$ (stored energy $\varepsilon = \vec{M} \cdot \vec{B}$ then $\vec{F} = \vec{\nabla}\varepsilon$)

Expand $\vec{M} = M_x \hat{x} + M_y \hat{y} + M_z \hat{z}$

Then $\vec{F} = \vec{\nabla}\left[M_x B_x + M_y B_y + M_z B_z\right]$

Design and apparatus in which $B = B_z$ is in the $\hat{z}$ direction only

Then $\vec{F} = \vec{\nabla}\left[M_z B_z\right]$

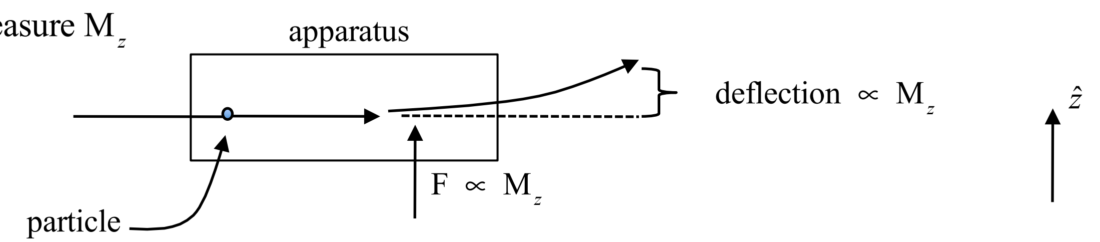
Since M is a fundamental property of a particle, it has no dependence on z

To get $\vec{\nabla}\left[M_z B_z\right] \neq 0$, must have $B_z = f(z)$

Then $F = M_z \frac{\partial B}{\partial z}$

Now if a particle with moment M_z is in the apparatus, it will feel a force $\propto M_z$.

If the particle is moving through the apparatus, the force will deflect its path from a straight line and its deflection will measure M_z



An apparatus like this is called a Stern-Gerlach Experiment

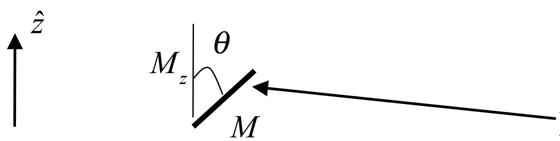
Notice that if you pass 1 particle through the SG, you find out its specific M_z.

If you accumulate a large number of identical particles, you can find out what are all the possible M_z values that they can have.

Recall m can take only quantized values. But are there any restrictions on M_z ?

$\propto$ the apparent orientation of the object

$$M_z = m\cos\theta$$



particle's magnetic dipole

Stern and Gerlach mad a beam of silver atoms.

For each atom
- the nucleus has $\vec{M} \approx 0$
- all e^- but the outermost one are paired, so their cumulative $\vec{M} \approx 0$
- the outermost e was in the s-suborbital of its shell

ℓ=0,

m=0

- the atoms were cooled so that it was unlikely the outermost e^- could acquire enough thermal energy to move a $\left\{\begin{matrix}\text{higher -}\ell \\ \text{higher m}\end{matrix}\right\}$ sub-orbital

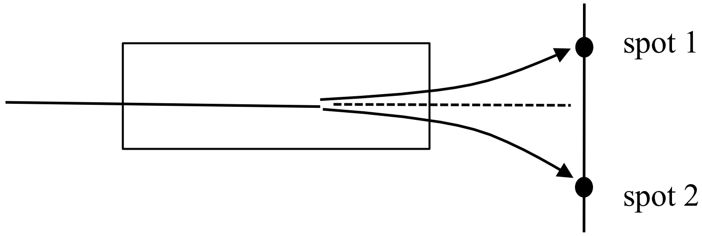
When the atoms passed through the SG, they all deflected, but each ended up in one of only 2 possible spots:

I. The Discovery of Spin

II. Filtering particles with a Stern-Gerlach apparatus

III. Experiments with filtered atoms

Read handout from Feynman lectures and Chapter 15



(smear that didn't appear)

What this meant:

1. the $\vec{M}$ cannot have arbitrary orientation: otherwise instead of 2 spots there would have been a continuous smear reflecting that all possible M_z states were present
2. each outer e^- had a non-zero M_z which was not related to its $\underbrace{\text{orbital angular momentum}}_{\text{that had been arranged to have } \ell=m=0}$

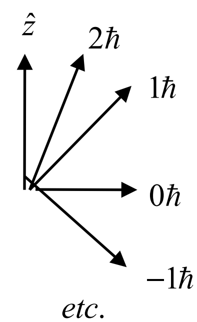
   call this "non-orbital angular momentum" = spin. Its quantum number is s
   and its "orbital angular momentum" $m = m_s$
3. Recall for orbital angular momentum, the possible values m can take are $-\ell,\ \ell+1,\ \ldots,\ 0,\ \ldots,\ \ell-1,\ \ell$
   so the number of possible values of m is $(2\ell+1)$
4. here, experimentally it was found that the number of possible m_s values is 2
   so $(2s+1) = 2$

$$\downarrow$$

$$s = \tfrac{1}{2}$$

*Conclusion: Every particle has, in addition to orbital angular momentum, another property which is mathematically like angular momentum but which is not due to any kind of rotation.
This new kind of angular momentum is called spin.

Recall that regular angular momentum is quantized in the direction its allowed to have, so that



$L_z =$ (integer m)*$\hbar$

the possible number of orientations is $2\ell+1$

m_{sz} is also quantized, but since s for an e^- is always $\frac{1}{2}$,

the number of possible m_s orientations is always only 2:

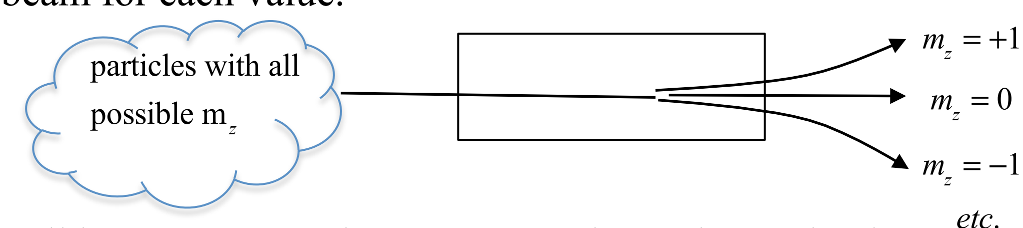
$+\frac{1}{2}$ and $-\frac{1}{2}$

I. Filtering particles with a Stern-Gerlach apparatus

quantum # m

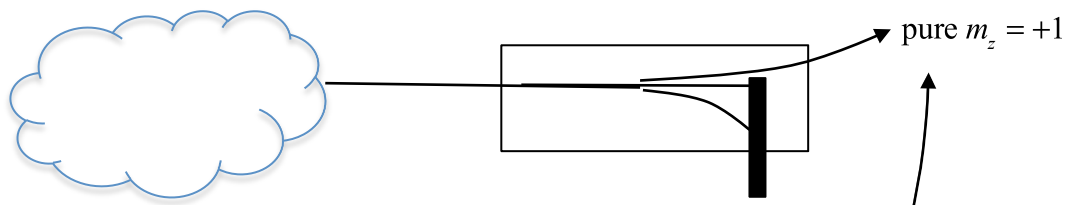
if their ℓ=0 this is due to their spin z

Recall if you have a collection of atoms with different m_z values, if you pass them through a Stern-Gerlach device, they will separate into different beams, one beam for each value.



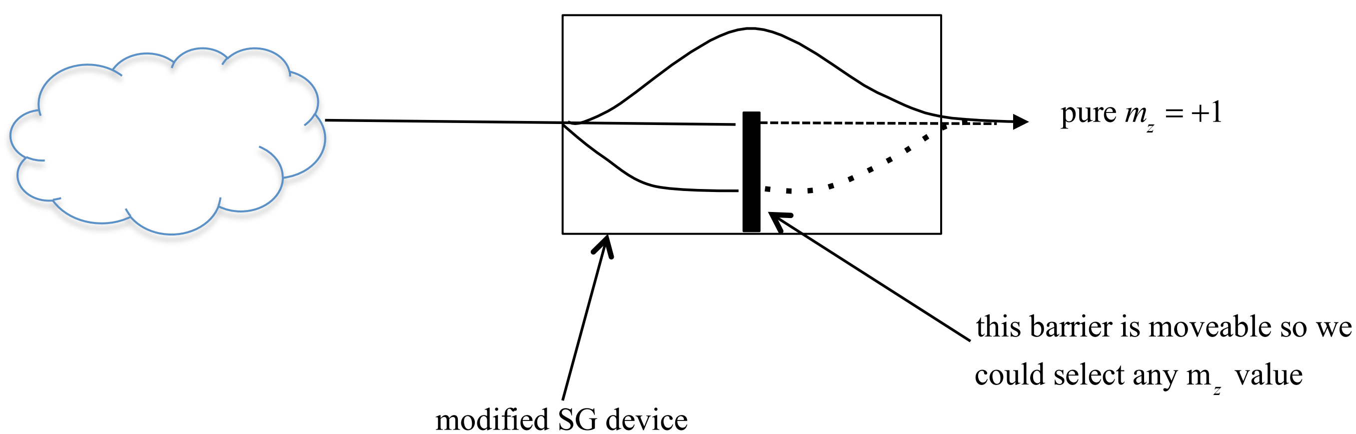
Notice if you obstruct all but 1 output path, you can produce a beam that is purely composed of particles with 1 definite m_z value.

Example:



When a beam is put into a definite state like this,
it (the output of the SG) is called a "prepared beam"
or a "filtered beam" or a "polarized beam"

Now make a slightly modified SG that can return the polarized beam
to the original axis of travel



Make up a symbol for the modified SG device:

$$\left\{\begin{array}{cc} +1 & \\ 0 & \blacksquare \\ -1 & \blacksquare \end{array}\right\} \leftarrow \text{this shows what is blocked}$$

S ← this gives a particular device a name in case more than 1 is in series

Make up symbols for the $\underbrace{\text{prepared states:}}_{\text{what come out of S}}$

|+ >

|0 >

|- >

Now imagine placing several SG's in series.

Example:

$$\text{beam} \rightarrow \underset{S}{\left\{\begin{array}{cc} +1 & \\ 0 & \blacksquare \\ -1 & \blacksquare \end{array}\right\}} \underset{S'}{\left\{\begin{array}{cc} +1 & \blacksquare \\ 0 & \blacksquare \\ -1 & \end{array}\right\}}$$

*Note S can represent both the device that prepares a particle's state, or the state itself

If this S is the initial state we are forcing the particles to have (labelled |+ >, etc.) then this S′ is the final state we are checking to see IF they have label final states with bras.

This one is < -1|

Other possibilities for this system are < 0 | or < +1|

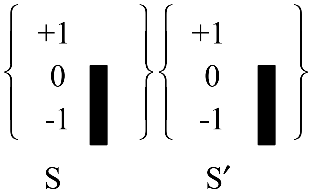
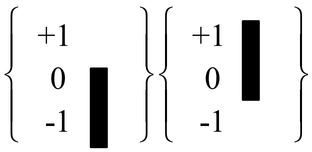
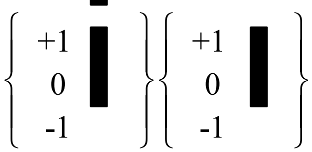
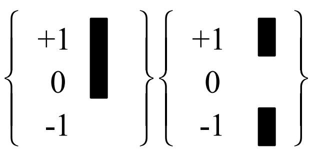
I. Filtering particles with a SG (continued)

II. Experiments with filtered atoms

III. SG in series

IV. Basis states and interference

Examples of some diferent possible results of putting 2 SG's in series:

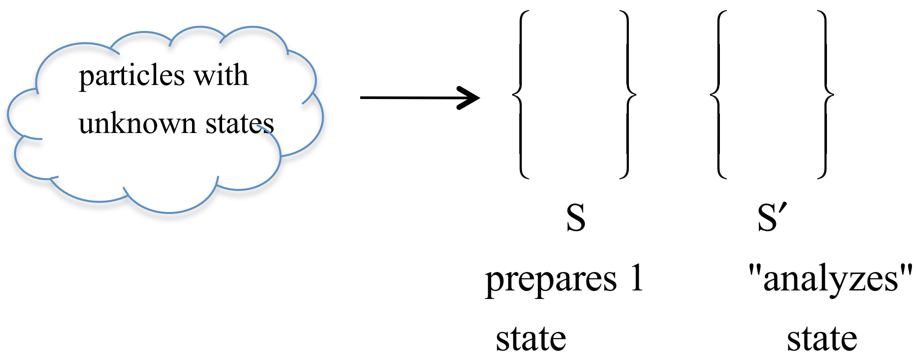
Configuration:	Result exiting S′	A symbolic way to represent this:
beam → 	all the pure $m_z = +1$ exit	$\left\langle \begin{matrix}\text{final}\\ \text{state}\end{matrix} \middle\vert \begin{matrix}\text{initial}\\ \text{state}\end{matrix} \right\rangle$ = fraction S that pass S $\langle +1 \vert +1 \rangle = 1$
beam → 	nothing exits	$\langle -1 \vert +1 \rangle = 1$
beam → 	all the pure $m_z = -1$ exit	$\langle -1 \vert -1 \rangle = 1$
beam → 	nothing exits	$\langle 0 \vert -1 \rangle = 1$

*Notice we draw the S, S′ in the order in which the beam reaches them, but we order $\langle \text{final} \vert \text{initial} \rangle$ from right to left.

We could summarize all possibilities in a matrix as we have done before:

final state	initial state: $\vert +1\rangle$	$\vert 0\rangle$	$\vert -1\rangle$
$\langle +1 \vert$	1	0	0
$\langle 0 \vert$	0	1	0
$\langle -1 \vert$	0	0	1

All these examples have



Suppose S could prepare several states with definite fractions, so

$$\left|\text{initial}\right\rangle = a\left|+\right\rangle + b\left|0\right\rangle + c\left|-\right\rangle$$

Then the amplitude for having a particular *final* state exit would be

$$\left\langle\text{final}\middle|\text{initial}\right\rangle = a\left\langle\text{final}\middle|+\right\rangle + b\left\langle\text{final}\middle|0\right\rangle + c\left\langle\text{final}\middle|-\right\rangle$$

$$= a \text{ if final} = \left\langle+1\right|$$

$$= \text{b if final} = \left\langle 0\right|$$

$$= \text{c if final} = \left\langle-1\right|$$

Then the *probability* of observing a particular final state is

$$\left|\left\langle\text{final}\middle|\text{initial}\right\rangle\right|^2 = |a|^2,\ |b|^2,\text{ or }|c|^2$$

We always assume that $\displaystyle\sum_{\text{final}}\left|\left\langle\text{final}\middle|\text{initial}\right\rangle\right|^2 = 1$

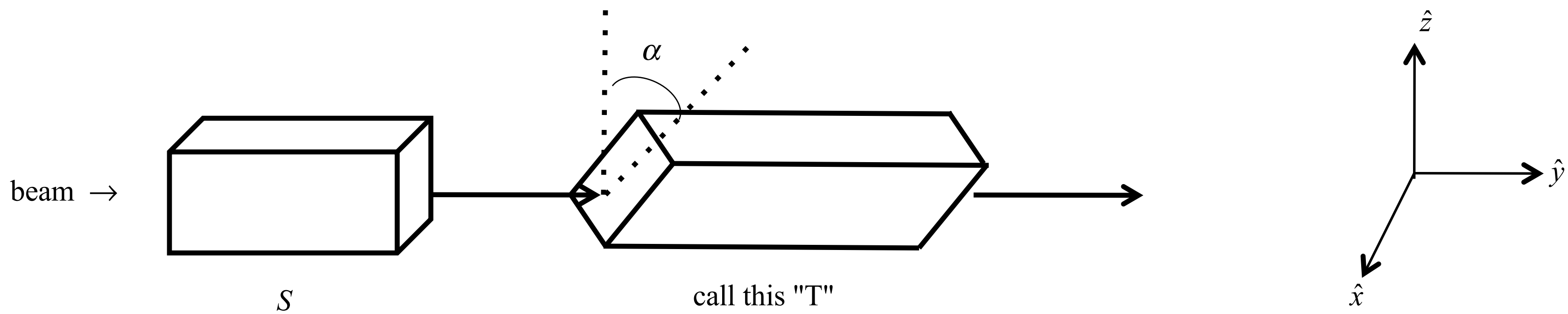
$$|a|^2 + |b|^2 + |c|^2 = 1$$

(This is normalization.)

II. Experiments with filtered atoms

The purpose of these examples is to show you how different basis sets could actually be realized in nature.

Suppose we put 2 SG filters in series, but one is tilted with respect to the other:



$|+S\rangle \neq |+T\rangle$, so $\langle +T|+S\rangle \neq 1$

However, since $|+S\rangle$ is not orthogonal to $|+T\rangle$, it is also not true that $\langle +T|+S\rangle = 0$

It turns out that $\langle +T|+S\rangle =$ some amplitude "a" where $0 \leq$ a ≤ 1 and a=f(α)

There are also specific amplitudes for all of the following possibilities:

$\langle +T|+S\rangle \quad \langle +T|0S\rangle \quad \langle +T|-S\rangle$

$\langle 0T|+S\rangle \quad \langle 0T|0S\rangle \quad \langle 0T|-S\rangle$

$\langle -T|+S\rangle \quad \langle -T|0S\rangle \quad \langle -T|-S\rangle$

Note: for normalization, the square of the $\langle 1\rangle$ in each column must sum to 1.

Keep in mind that the matrix of possibilities does not have to be 3x3. It is in general nxn, where n is the number of states the beam particles can have.

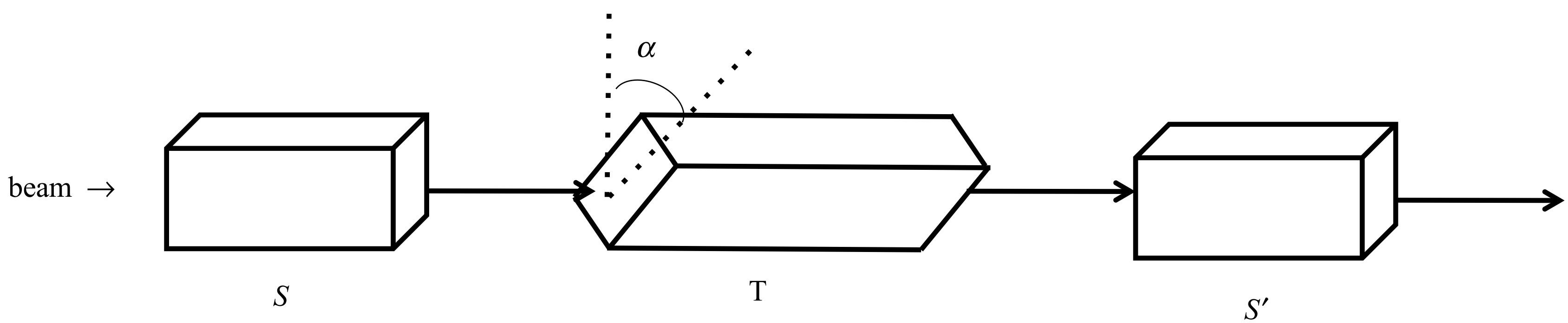
III. SG filters in series

The message of this section is,

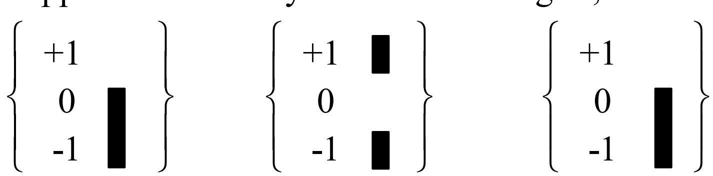
once a particle goes through a filter it loses all information about the orientation of previous filters it passes through.
That is not the same as saying, "each filter analyzes, or *measures* the state of the particle, and the measurement process places the particle in and *eigenstate* of that measurement"

aligned along one of its basis states   of that SG filter

To see this, consider 3 consecutive SG filters:



Suppose the not only have relative angles, but also have their blocking pads in different places:



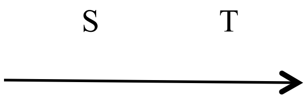
Notice S and S′ represent the same basis (which has 3 states), and T is a different one (which also has 3 states).

I. SG filters in series (continued)

II. Basis states and interference

III. Describing a measurement matrix

You might guess that a particle got to here,

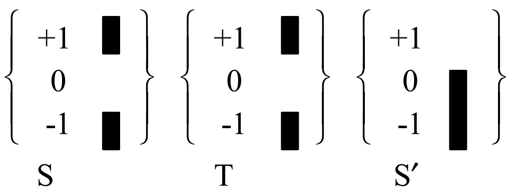


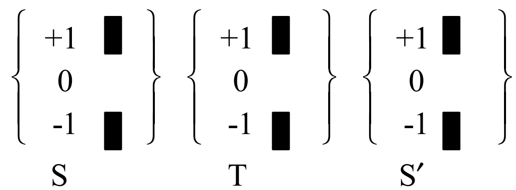
it would get to here

with 100% probability, because it would "remember" that is had been $\left|+S\right\rangle$ earlier. It does NOT.
The T filter places it into a $\left|0T\right\rangle$ state, which does *not* have 100% overlap with a $\left|+S\right\rangle$.

Demonstrate that the fraction of particles that pass through T and S′ depends only on T and S′ (not S)

Compare:





Amplitude to exit S′ is:

$\left\langle +S' \middle| 0T \right\rangle \left\langle 0T \middle| 0S \right\rangle$

$\left\langle 0S' \middle| 0T \right\rangle \left\langle 0T \middle| 0S \right\rangle$

Ratio of amplitudes is:

$$\frac{LHS}{RHS} = \frac{\left\langle +S' \middle| 0T \right\rangle \cancel{\left\langle 0T \middle| 0S \right\rangle}}{\underbrace{\left\langle 0S' \middle| 0T \right\rangle}_{\text{independent of state of S.}} \cancel{\left\langle 0T \middle| 0S \right\rangle}}$$

I. Basis states and interference

II. Describing a measurement with a matrix

III. Sequential measurements

Read Goswami 11.2

So the presence of S affects the absolute number of particles that get to T (and then have the chance to reach S′), but once they are at T, having passed through S does not affect their chance to pass through S′.

IV. Basis states and interference

Consider several experiments:

Experiment 1:

Experiment 2:

Experiment 3:

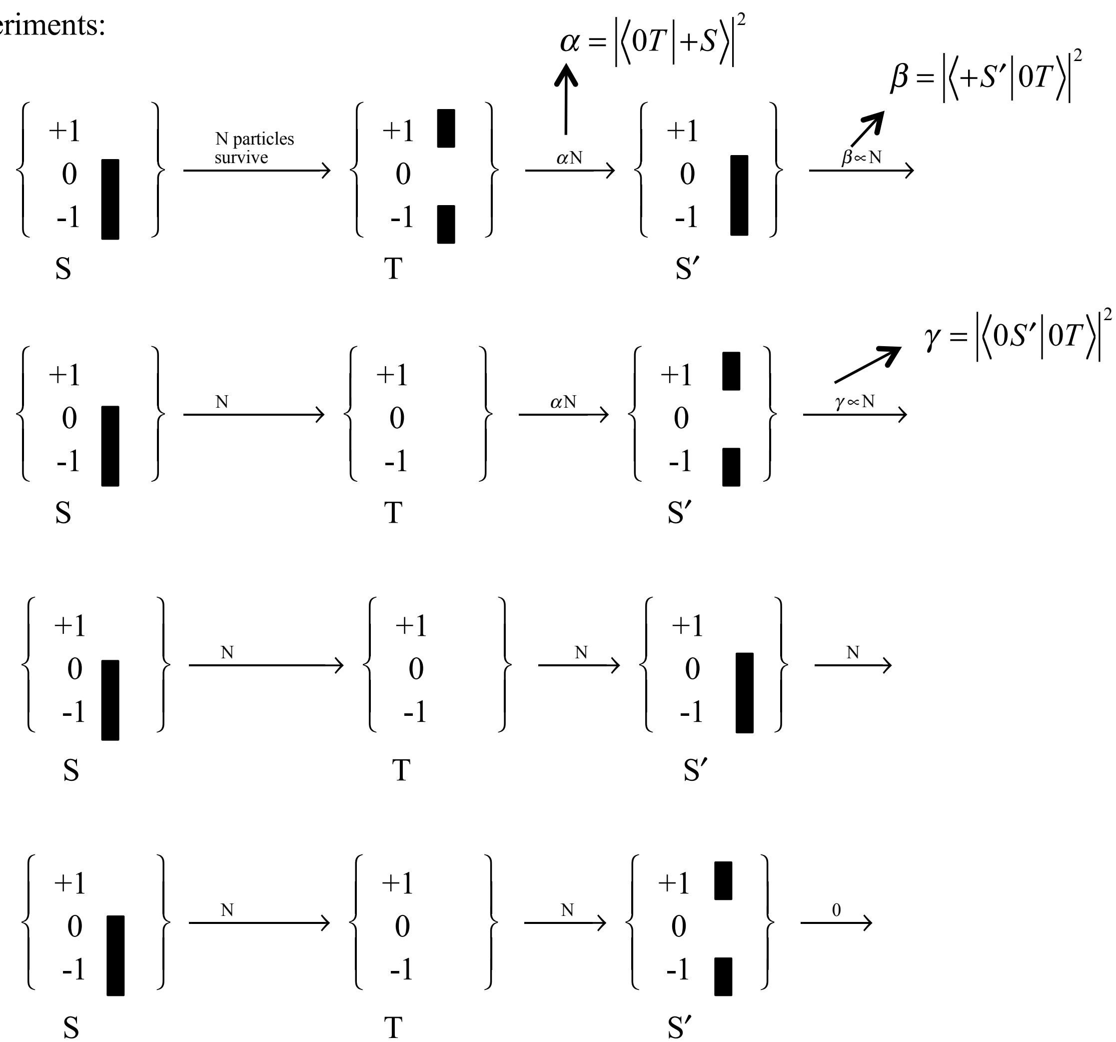
repeat Exp. 1 but

remove blocks from T

Experiment 4:

repeat Exp. 2 but

remove blocks from T

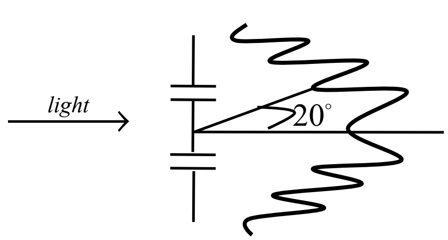


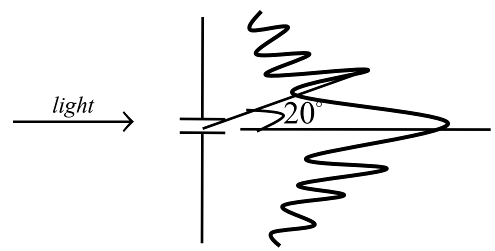
Conclusions:

• Experiment 2 produces more final state particles than Experiment 4:
Inserting blocks in T must eliminate destructive interference (or produce constructive interference) in this case.

• Experiment 1 produces *less* than Experiment 3:
Inserting blocks in Tmust produce destructive interference in this case.

This interference of amplitudes is similar to what happens in a double slit experiment with light:





2 slits
(like "no blocks" in T)
gives minimum
output at 20°

1 slit
(loss of one slit like adding a block in T)
gives maximum
output at 20°

Write the amplitudes:

Experiment 4: $\langle 0S'|+T\rangle\langle +T|+S\rangle$

$+ \ \langle 0S'|0T\rangle\langle 0T|+S\rangle$

$+ \ \langle 0S'|-T\rangle\langle -T|+S\rangle$

0

Experiment 3: $\langle +S'|+T\rangle\langle +T|+S\rangle$

$+ \ \langle +S'|0T\rangle\langle 0T|+S\rangle$

$+ \ \langle +S'|-T\rangle\langle -T|+S\rangle$

1

Condense the rotation:

$$\sum_{\text{all T}}\langle 0S'|+T\rangle\langle +T|+S\rangle = 0$$

$$\sum_{\text{all T}}\langle +S'|+T\rangle\langle +T|+S\rangle = 1$$

Facts about all of this:

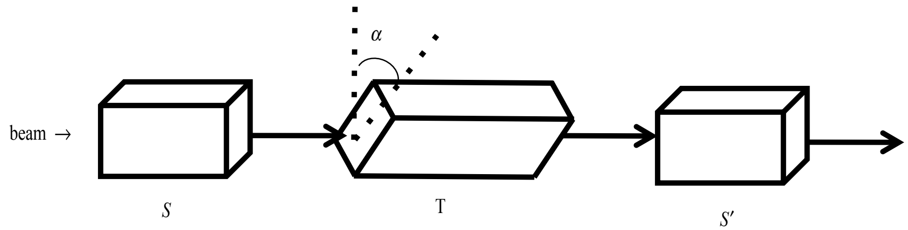
1. Experiment 3 would have the same result if
T is present but all open or T is not present at all

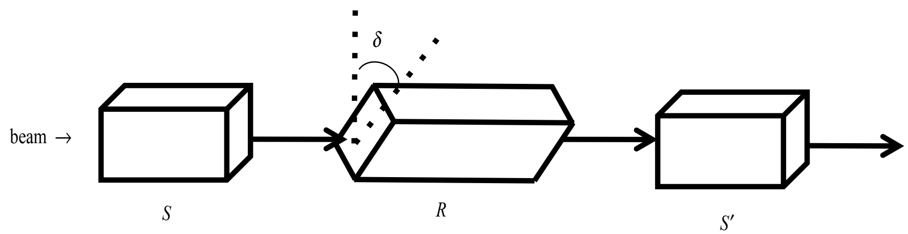
$$\sum_{\text{T}}\langle 0S'|T\rangle\langle T|+S\rangle = \langle 0S'|+S\rangle$$

$\Rightarrow$ So $\sum_{T}|T\rangle\langle T| = 1$ If T includes $\underbrace{\text{all possible imtermediate states}}_{\text{it is a basis, a complete set}}$

2. Experiment 3 would have the same result if T were replaced by some other filter "R" tipped at an angle other than α, as long as R were also unblocked.

Now





$\Rightarrow$ So a choice of basis is not unique.

3. All of this only works if the states within a basis are orthogonal, for example $\langle T_i | T_j \rangle = \delta_{ij}$

To see this, go back to

$$\sum_T \langle 0S' | T \rangle \langle T | +S \rangle = \langle 0S | +S \rangle$$

$\downarrow$

Note that S′ and S are really the same basis, so delete the prime

$$\sum_T \langle 0S | T \rangle \langle T | +S \rangle = \langle 0S | +S \rangle$$

$\downarrow$

Rename $|+S\rangle = |\phi\rangle$ generic

$\langle 0S| = |\chi\rangle$ generic

$|T\rangle\langle T| = |i\rangle\langle i|$ any basis

$$\sum_i \langle \chi | i \rangle \langle i | \phi \rangle = \langle \chi | \phi \rangle$$

Now since $|\phi\rangle$ is generic, it could be a member of the basis set, $|j\rangle$

$$\sum_i \langle \chi | i \rangle \langle i | j \rangle = \langle \chi | j \rangle$$

This can only be true if $\langle i | j \rangle = \delta_{ij}$

4. Revising the order of a process (i.e. exchanging the initial and final states) is the same as taking the complex conjugate of its amplitude.

Show this:

2 columns:

Column 1:

If a particle starts in some state, it must end up in one of the possible final states (i.e. it cannot get lost).

So, for example:

$$|\langle +T | +S \rangle|^2 + |\langle 0T | +S \rangle|^2 + |\langle -T | +S \rangle|^2 = 1$$

Expand:

$$\langle +T | +S \rangle^* \langle +T | +S \rangle + \langle 0T | +S \rangle^* \langle 0T | +S \rangle + \langle -T | +S \rangle^* \langle -T | +S \rangle = 1$$ "Equation A"

Column 2:

Now also recall that if a state (say $|+S\rangle$) is normalized, for example:

$$\langle +S | +S \rangle = 1$$

$\downarrow$

we can insert $\sum_T |T\rangle\langle T| = 1$

I. Describing a measurement with a matrix

II. Sequential measurements

III. Relating matrix notation and Dirac notation

IV. Spinors

Example:

Suppose:

$\left|+S\right\rangle =$ an electron

A = and interaction or measurement

$\left\langle +R\right| =$ and up quark

Finding $\left\langle +R\right| A \left|+S\right\rangle$ tells us the probability that this interaction converts e $\rightarrow$ w, which is fundamental information about the interaction.

$$\sum_T \langle +S|T\rangle\langle T|+S\rangle = 1$$

$$\downarrow$$

$$\langle +S|+T\rangle\langle +T|+S\rangle + \langle +S|0T\rangle\langle 0T|+S\rangle + \langle +S|-T\rangle\langle -T|+S\rangle = 1 \qquad \text{"Equation B"}$$

Compare Equation A and Equation B

Both have RHS=1, so their LHS's must be equal.

This can only be true if

$$\boxed{\langle S_i|T_j\rangle = \langle T_j|S_i\rangle^*}$$

V. Describing a measurement by a matrix

Common question in physics:

- A system begins in some initial state, say $|+S\rangle$ (The full set of possible states is "S")
- Something happens to it (a measurement--call it "A" or and interaction force)
- What is the probability that it will end up in any particular final state, say $\langle +R|$ (the full set of possible final states is "R")

So we want $\langle +R|A|+S\rangle$. (see previous page)

How to calculate this?

Here $|+S\rangle$ and $\langle +R|$ are bras and kets in Hilbert space, it is hard to calculate with them without choosing a basis.

But what basis is best for them? What if calculating with each are easier if they are in different basis?

(This could happen, for example, if $|+S\rangle$ is a state with rectangular symmetry and $\langle +R|$ is a state with spherical symmetry.)

How to handle this:

We have:

$$\langle +R|A|+S\rangle = \underset{S}{\begin{Bmatrix} +1 \\ 0 \\ -1 \end{Bmatrix}} \begin{Bmatrix} A \end{Bmatrix} \underset{R}{\begin{Bmatrix} +1 \\ 0 \\ -1 \end{Bmatrix}}$$

Inserting an unblocked $\begin{Bmatrix} T \end{Bmatrix}$ anywhere has no effect:

So

$$\langle +R|A|+S\rangle = \underset{S}{\begin{Bmatrix} +1 \\ 0 \\ -1 \end{Bmatrix}} \underset{T}{\begin{Bmatrix} +1 \\ 0 \\ -1 \end{Bmatrix}} \begin{Bmatrix} A \end{Bmatrix} \underset{T}{\begin{Bmatrix} +1 \\ 0 \\ -1 \end{Bmatrix}} \underset{R}{\begin{Bmatrix} +1 \\ 0 \\ -1 \end{Bmatrix}}$$

Make a table:

The amplitude for going from

$+S \rightarrow T$ $\quad$ $T \rightarrow A \rightarrow T$ $\quad$ $T \rightarrow +R$

is given by

$\langle T_i|+S\rangle$ $\quad$ $\sum_i \langle T_j|A|T_i\rangle$ $\quad$ $\sum_j \langle +R|T_j\rangle$

I. Describing a measurement matrix (continued)

II. Sequential measurements

III. Relating matrix notation to Dirac notation

Reordering:

$$\langle +R|A|+S\rangle = \sum_{ij} \langle +R|T_j\rangle\langle T_j|A|T_i\rangle\langle T_i|+S\rangle$$

Rename $|+S\rangle = |\phi\rangle$ generic state

$\langle +R| = \langle \chi|$ generic state

$|T_i\rangle,\ |T_j\rangle \rightarrow |i\rangle,\ |j\rangle$ members of any basis

Then

$$\boxed{\langle \chi|A|\phi\rangle = \sum_{i,j} \langle \chi|j\rangle\langle j|A|i\rangle\langle i|\phi\rangle}$$

What this means:

Suppose that $|\phi\rangle$ and $|\chi\rangle$ can be written in terms of bases with 3 basis states.

Then i=(1,2,3) and j=(1,2,3)

So there are only 9 possible amplitudes $\langle j|A|i\rangle$

For example:

i→ j↓	+	0	-
+	$\langle +\|A\|+\rangle$	$\langle +\|A\|0\rangle$	$\langle +\|A\|-\rangle$
0	$\langle 0\|A\|+\rangle$	$\langle 0\|A\|0\rangle$	$\langle 0\|A\|-\rangle$
-	$\langle -\|A\|+\rangle$	$\langle -\|A\|0\rangle$	$\langle -\|A\|-\rangle$

(Notice order the columns and rows in descending order of the eigenvalues of the quantum number involved.)

And there are only 3 amplitudes $\langle i|\phi\rangle$

And there are only 3 amplitudes $\langle\chi|j\rangle$

So a total of 9+3+3=15 pieces of information are required.

Once they are plugged into the sum of the RHS, you get the LHS, which is a very general peice of information: "How does the $\underbrace{\text{measurement}}_{\text{operator}}$ A relate the states $|\phi\rangle$ and $\langle\chi|$?"

VI. Sequential measurements

Suppose "measurement A" really involves "first measure B, then C"

Example: to find out the mass of a fundamental particles you could measure first its $\vec{p}$, then its $\vec{v}$, then calculate m=$\frac{p}{v}$

Get p from tracking the curvature of its path in a $\vec{B}$ field:

curvature k $\propto \frac{B}{p}$

Then get $\vec{v}$ by putting it through a "speed trap": measure its times t_1 and t_2 crossing 2 points separated by length l, then compute v=$\frac{l}{t_2 - t_1}$

So procedurally the measurement would be:

$$\underset{\phi}{\{\ \}} \rightarrow \{A\} \rightarrow \underset{\chi}{\{\ \}} = \underset{\phi}{\{\ \}} \rightarrow \{B\} \rightarrow \{C\} \rightarrow \underset{\chi}{\{\ \}}$$

$$\underset{\phi}{\{\ \}}\{A\}\underset{\chi}{\{\ \}} = \underset{\phi}{\{\ \}}\{B\}\underset{\mathrm{T}}{\{\ \}}\{C\}\underset{\chi}{\{\ \}}$$

Symbolically:

$$\langle \chi | A | \phi \rangle = \sum_{T_j} \langle \chi | C | T_j \rangle \langle T_j | B | \phi \rangle$$ notice generator order is right-to-left

since T_j unblocked

each of these is a matrix in which the ket=initial state labels columns
bra= final state, labels rows
The sum over the $|T_j\rangle\langle T_j|$ represents the normal procedure for matrix multiplication.

Show this:
In normal $\overbrace{\text{matrix multiplication}}^{A = B\cdot C}$ the (χ,ϕ)th element of matrix A is the sum of the element-by-element product of the matrix elements in the χ-th row of B and the ϕ-th row of C:

Example: for χ=2, ϕ=3

$$\begin{pmatrix} (1,1) & (1,2) & (1,3) & \ldots & (1,5) \\ (2,1) & (2,2) & (2,3) & \ldots & (2,5) \\ \vdots & & & & \\ \vdots & & & & \\ (5,1) & (5,2) & (5,3) & \ldots & (5,5) \end{pmatrix} = \begin{pmatrix} \\ (2,1) & (2,2) & (2,3) & (2,4) & (2,5) \\ \\ \\ \end{pmatrix} \bullet \begin{pmatrix} (1,3) \\ (2,3) \\ (3,3) \\ (3,4) \\ (3,5) \end{pmatrix}$$

matrix A matrix B matrix C

$$\mathrm{A}_{23} = B_{21}C_{13} + B_{22}C_{23} + B_{23}C_{33} + B_{24}C_{43} + B_{25}C_{53} = \sum_{T_j} B_{2T_j} C_{T_j 3}$$

I. Relating matrix notation and Dirac notation

Recall we have

initial state = $|i\rangle$

finale state = $\langle f|$

operator = A

Then

$\langle f|A|i\rangle$ means:

- something ("A") is close to state $|i\rangle$
- that event changes the state to something else (call is state $|A_i\rangle$)
- we want to know $\boxed{\text{how } |A_i\rangle \text{ compares to the state } \langle f|}$
- the overlap of them is given by $\langle f|A_i\rangle$

$$\Updownarrow$$

$$\langle f|A|i\rangle$$

Another way to say this is "what is the probablility that $|A_i\rangle$ is identical to $|f\rangle$?"

Now recall that since the elements $|\alpha\rangle$ of a basis are complete,

$$\sum_{\alpha} |\alpha\rangle\langle\alpha| = 1$$

This is true for any basis so also true for the basis $|\beta\rangle$

$$\sum_{\beta} |\beta\rangle\langle\beta| = 1$$

This allows is to write

$$\underbrace{\langle f|A|i\rangle} = \sum_{\alpha}\sum_{\beta} \underbrace{\langle f|\beta\rangle}\underbrace{\langle\beta|A|\alpha\rangle}\underbrace{\langle\alpha|i\rangle}$$

Recall that this symbol means "Hilbert space state $|i\rangle$ projected into the $|\alpha\rangle$ basis"

Recall that these are matrices

Recall $\langle f|\beta\rangle = \langle\beta|f\rangle^*$
so this is the complex conjugate
of Hilbert space state $|f\rangle$
projected into the $|\beta\rangle$ basis.

Example: Suppose that $|i\rangle$ and $|f\rangle$ can each take on 3 values. (Ex: +1, 0, -1)

Then

- $\langle f|A|i\rangle$ is a 3x3 matrix
- if the $|\alpha\rangle$'s span the space in which $|i\rangle$ exists there need be only 3 values of $|\alpha\rangle$
- if the $|\beta\rangle$'s span the space in which $|f\rangle$ exists there need be only 3 values of $|\beta\rangle$

I. Spinors

II. The matrices and eigenspinors of S_x and S_y

So the equation looks like

$$\underbrace{\langle f|A|i\rangle}_{\text{3x3}} = \sum_{\alpha,\beta} \underbrace{\langle f|\beta\rangle}_{\text{3-component vector}} \underbrace{\langle \beta|A|\alpha\rangle}_{\text{3x3}} \underbrace{\langle \alpha|i\rangle}_{\text{3-component vector}}$$

Normal rules of matrix multiplication state that the $\underbrace{\text{vector to the right}}_{\langle \alpha|i\rangle}$ of the matrix must be a *column vector*

and the $\underbrace{\text{vector to the left}}_{\langle f|\beta\rangle}$ of the matrix must be a *row vector*

So translating from Dirac notation to matrix notation gives:

$$\underbrace{\begin{pmatrix} \quad & \quad & \quad \\ & & \\ & & \end{pmatrix}}_{\langle f|A|i\rangle} = \underbrace{\begin{pmatrix} \quad & \quad & \quad \end{pmatrix}}_{\langle f|\beta\rangle} \underbrace{\begin{pmatrix} \quad & \quad & \quad \\ & & \\ & & \end{pmatrix}}_{\langle \beta|A|\alpha\rangle} \underbrace{\begin{pmatrix} \quad \\ \\ \\ \end{pmatrix}}_{\langle \alpha|i\rangle}$$