34. CLEBSCH-GORDAN COEFFICIENTS, SPHERICAL HARMONICS, AND *d* FUNCTIONS

Note: A square-root sign is to be understood over *every* coefficient, *e.g.*, for −8/15 read $-\sqrt{8/15}$.

Notation:

		J	J	...
		M	M	...
m_1	m_2	Coefficients		
m_1	m_2			
.	.			
.	.			

1/2×1/2

		1
		+1
+1/2	+1/2	1

		1	0
		0	0
+1/2	−1/2	1/2	1/2
−1/2	+1/2	1/2	−1/2

		1
		−1
−1/2	−1/2	1

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}$$

$$Y_2^0 = \sqrt{\frac{5}{4\pi}}\Big(\frac{3}{2}\cos^2\theta - \frac{1}{2}\Big)$$

$$Y_2^1 = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{i\phi}$$

$$Y_2^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{2i\phi}$$

2×1/2

		5/2
		+5/2
+2	+1/2	1

		5/2	3/2
		+3/2	+3/2
+2	−1/2	1/5	4/5
+1	+1/2	4/5	−1/5

		5/2	3/2
		+1/2	+1/2
+1	−1/2	2/5	3/5
0	+1/2	3/5	−2/5

		5/2	3/2
		−1/2	−1/2
0	−1/2	3/5	2/5
−1	+1/2	2/5	−3/5

		5/2	3/2
		−3/2	−3/2
−1	−1/2	4/5	1/5
−2	+1/2	1/5	−4/5

		5/2
		−5/2
−2	−1/2	1

1×1/2

		3/2
		+3/2
+1	+1/2	1

		3/2	1/2
		+1/2	+1/2
+1	−1/2	1/3	2/3
0	+1/2	2/3	−1/3

		3/2	1/2
		−1/2	−1/2
0	−1/2	2/3	1/3
−1	+1/2	1/3	−2/3

		3/2
		−3/2
−1	−1/2	1

3/2×1/2

		2
		+2
+3/2	+1/2	1

		2	1
		+1	+1
+3/2	−1/2	1/4	3/4
+1/2	+1/2	3/4	−1/4

		2	1
		0	0
+1/2	−1/2	1/2	1/2
−1/2	+1/2	1/2	−1/2

		2	1
		−1	−1
−1/2	−1/2	3/4	1/4
−3/2	+1/2	1/4	−3/4

		2
		−2
−3/2	−1/2	1

2×1

		3
		+3
+2	+1	1

		3	2
		+2	+2
+2	0	1/3	2/3
+1	+1	2/3	−1/3

		3	2	1
		+1	+1	+1
+2	−1	1/15	1/3	3/5
+1	0	8/15	1/6	−3/10
0	+1	2/5	−1/2	1/10

		3	2	1
		0	0	0
+1	−1	1/5	1/2	3/10
0	0	3/5	0	−2/5
−1	+1	1/5	−1/2	3/10

		3	2	1
		−1	−1	−1
0	−1	2/5	1/2	1/10
−1	0	8/15	−1/6	−3/10
−2	+1	1/15	−1/3	3/5

		3	2
		−2	−2
−1	−1	2/3	1/3
−2	0	1/3	−2/3

		3
		−3
−2	−1	1

3/2×1

		5/2
		+5/2
+3/2	+1	1

		5/2	3/2
		+3/2	+3/2
+3/2	0	2/5	3/5
+1/2	+1	3/5	−2/5

		5/2	3/2	1/2
		+1/2	+1/2	+1/2
+3/2	−1	1/10	2/5	1/2
+1/2	0	3/5	1/15	−1/3
−1/2	+1	3/10	−8/15	1/6

		5/2	3/2	1/2
		−1/2	−1/2	−1/2
+1/2	−1	3/10	8/15	1/6
−1/2	0	3/5	−1/15	−1/3
−3/2	+1	1/10	−2/5	1/2

		5/2	3/2
		−3/2	−3/2
−1/2	−1	3/5	2/5
−3/2	0	2/5	−3/5

		5/2
		−5/2
−3/2	−1	1

1×1

		2
		+2
+1	+1	1

		2	1
		+1	+1
+1	0	1/2	1/2
0	+1	1/2	−1/2

		2	1	0
		0	0	0
+1	−1	1/6	1/2	1/3
0	0	2/3	0	−1/3
−1	+1	1/6	−1/2	1/3

		2	1
		−1	−1
0	−1	1/2	1/2
−1	0	1/2	−1/2

		2
		−2
−1	−1	1

$$Y_\ell^{-m} = (-1)^m Y_\ell^{m*}$$

$$d^{\,\ell}_{m,0} = \sqrt{\frac{4\pi}{2\ell+1}}\, Y_\ell^m\, e^{-im\phi}$$

$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 J M\rangle = (-1)^{J-j_1-j_2}\langle j_2 j_1 m_2 m_1 | j_2 j_1 J M\rangle$$

$$d^{\,j}_{m',m} = (-1)^{m-m'} d^{\,j}_{m,m'} = d^{\,j}_{-m,-m'}$$

3/2×3/2

		3
		+3
+3/2	+3/2	1

		3	2
		+2	+2
+3/2	+1/2	1/2	1/2
+1/2	+3/2	1/2	−1/2

		3	2	1
		+1	+1	+1
+3/2	−1/2	1/5	1/2	3/10
+1/2	+1/2	3/5	0	−2/5
−1/2	+3/2	1/5	−1/2	3/10

		3	2	1	0
		0	0	0	0
+3/2	−3/2	1/20	1/4	9/20	1/4
+1/2	−1/2	9/20	1/4	−1/20	−1/4
−1/2	+1/2	9/20	−1/4	−1/20	1/4
−3/2	+3/2	1/20	−1/4	9/20	−1/4

		3	2	1
		−1	−1	−1
+1/2	−3/2	1/5	1/2	3/10
−1/2	−1/2	3/5	0	−2/5
−3/2	+1/2	1/5	−1/2	3/10

		3	2
		−2	−2
−1/2	−3/2	1/2	1/2
−3/2	−1/2	1/2	−1/2

		3
		−3
−3/2	−3/2	1

$$d^{\,1}_{0,0} = \cos\theta \qquad d^{\,1/2}_{1/2,1/2} = \cos\frac{\theta}{2} \qquad d^{\,1}_{1,1} = \frac{1+\cos\theta}{2}$$

$$d^{\,1/2}_{1/2,-1/2} = -\sin\frac{\theta}{2} \qquad d^{\,1}_{1,0} = -\frac{\sin\theta}{\sqrt{2}}$$

$$d^{\,1}_{1,-1} = \frac{1-\cos\theta}{2}$$

2×3/2

		7/2
		+7/2
+2	+3/2	1

		7/2	5/2
		+5/2	+5/2
+2	+1/2	3/7	4/7
+1	+3/2	4/7	−3/7

		7/2	5/2	3/2
		+3/2	+3/2	+3/2
+2	−1/2	1/7	16/35	2/5
+1	+1/2	4/7	1/35	−2/5
0	+3/2	2/7	−18/35	1/5

		7/2	5/2	3/2	1/2
		+1/2	+1/2	+1/2	+1/2
+2	−3/2	1/35	6/35	2/5	2/5
+1	−1/2	12/35	5/14	0	−3/10
0	+1/2	18/35	−3/35	−1/5	1/5
−1	+3/2	4/35	−27/70	2/5	−1/10

		7/2	5/2	3/2	1/2
		−1/2	−1/2	−1/2	−1/2
+1	−3/2	4/35	27/70	2/5	1/10
0	−1/2	18/35	3/35	−1/5	−1/5
−1	+1/2	12/35	−5/14	0	3/10
−2	+3/2	1/35	−6/35	2/5	−2/5

		7/2	5/2	3/2
		−3/2	−3/2	−3/2
0	−3/2	2/7	18/35	1/5
−1	−1/2	4/7	−1/35	−2/5
−2	+1/2	1/7	−16/35	2/5

		7/2	5/2
		−5/2	−5/2
−1	−3/2	4/7	3/7
−2	−1/2	3/7	−4/7

		7/2
		−7/2
−2	−3/2	1

2×2

		4
		+4
+2	+2	1

		4	3
		+3	+3
+2	+1	1/2	1/2
+1	+2	1/2	−1/2

		4	3	2
		+2	+2	+2
+2	0	3/14	1/2	2/7
+1	+1	4/7	0	−3/7
0	+2	3/14	−1/2	2/7

		4	3	2	1
		+1	+1	+1	+1
+2	−1	1/14	3/10	3/7	1/5
+1	0	3/7	1/5	−1/14	−3/10
0	+1	3/7	−1/5	−1/14	3/10
−1	+2	1/14	−3/10	3/7	−1/5

		4	3	2	1	0
		0	0	0	0	0
+2	−2	1/70	1/10	2/7	2/5	1/5
+1	−1	8/35	2/5	1/14	−1/10	−1/5
0	0	18/35	0	−2/7	0	1/5
−1	+1	8/35	−2/5	1/14	1/10	−1/5
−2	+2	1/70	−1/10	2/7	−2/5	1/5

		4	3	2	1
		−1	−1	−1	−1
+1	−2	1/14	3/10	3/7	1/5
0	−1	3/7	1/5	−1/14	−3/10
−1	0	3/7	−1/5	−1/14	3/10
−2	+1	1/14	−3/10	3/7	−1/5

		4	3	2
		−2	−2	−2
0	−2	3/14	1/2	2/7
−1	−1	4/7	0	−3/7
−2	0	3/14	−1/2	2/7

		4	3
		−3	−3
−1	−2	1/2	1/2
−2	−1	1/2	−1/2

		4
		−4
−2	−2	1

$$d^{\,3/2}_{3/2,3/2} = \frac{1+\cos\theta}{2}\cos\frac{\theta}{2}$$

$$d^{\,3/2}_{3/2,1/2} = -\sqrt{3}\frac{1+\cos\theta}{2}\sin\frac{\theta}{2} \qquad d^{\,2}_{2,2} = \Big(\frac{1+\cos\theta}{2}\Big)^2$$

$$d^{\,3/2}_{3/2,-1/2} = \sqrt{3}\frac{1-\cos\theta}{2}\cos\frac{\theta}{2} \qquad d^{\,2}_{2,1} = -\frac{1+\cos\theta}{2}\sin\theta$$

$$d^{\,3/2}_{3/2,-3/2} = -\frac{1-\cos\theta}{2}\sin\frac{\theta}{2} \qquad d^{\,2}_{2,0} = \frac{\sqrt{6}}{4}\sin^2\theta \qquad d^{\,2}_{1,1} = \frac{1+\cos\theta}{2}(2\cos\theta-1)$$

$$d^{\,3/2}_{1/2,1/2} = \frac{3\cos\theta-1}{2}\cos\frac{\theta}{2} \qquad d^{\,2}_{2,-1} = -\frac{1-\cos\theta}{2}\sin\theta \qquad d^{\,2}_{1,0} = -\sqrt{\frac{3}{2}}\sin\theta\cos\theta$$

$$d^{\,3/2}_{1/2,-1/2} = -\frac{3\cos\theta+1}{2}\sin\frac{\theta}{2} \qquad d^{\,2}_{2,-2} = \Big(\frac{1-\cos\theta}{2}\Big)^2 \qquad d^{\,2}_{1,-1} = \frac{1-\cos\theta}{2}(2\cos\theta+1) \qquad d^{\,2}_{0,0} = \Big(\frac{3}{2}\cos^2\theta - \frac{1}{2}\Big)$$

Figure 34.1: The sign convention is that of Wigner (*Group Theory*, Academic Press, New York, 1959), also used by Condon and Shortley (*The Theory of Atomic Spectra*, Cambridge Univ. Press, New York, 1953), Rose (*Elementary Theory of Angular Momentum*, Wiley, New York, 1957), and Cohen (*Tables of the Clebsch-Gordan Coefficients*, North American Rockwell Science Center, Thousand Oaks, Calif., 1974). The coefficients here have been calculated using computer programs written independently by Cohen and at LBNL.

PH431 : QUANTUM MECHANICS

Prof : Kelly Patton

Sep 4, 2019

3 historical stories

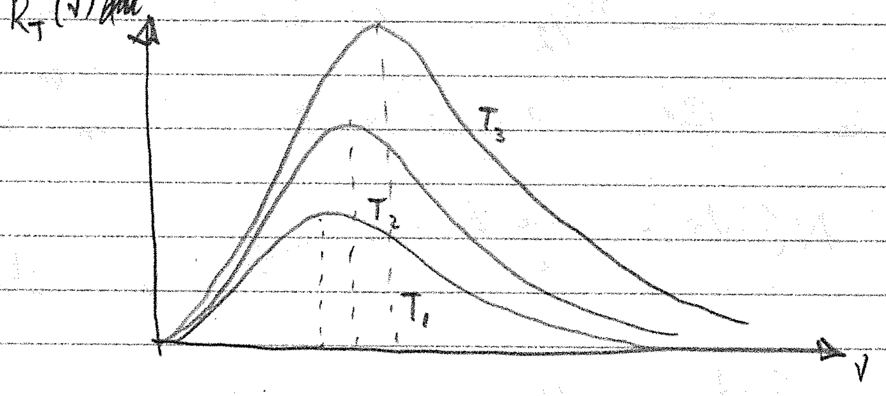
- Blackbody Radiation
- Waves vs. Particles
- Atomic Spectra

☒ Thermal radiation : radiation emitted by temperature, spectra independent of material.

↳ Blackbody : absorbs all radiation incident on them. Two blackbodies at same temp produce the same spectrum.

- Spectral distribution $\longrightarrow R_T(\nu)\,d\nu \rightarrow$ energy/time/area emitted between ν, $\rightarrow \nu + d\nu$

- Radiancy $\longrightarrow \int_0^\infty R_T(\nu)\,d\nu = R_T$



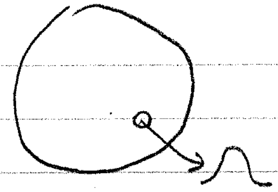
- Stefan – Boltzmann law

$$\int_0^\infty R_T(\nu)d\nu \longleftarrow R_T \sim \sigma T^4 \quad \text{where } \sigma = 5.67 \times 10^{-8}\ W/m^2K^4$$

- Wien's law $\left\{ \begin{array}{l} R_T \uparrow \text{ as } T \uparrow \\ \nu_{max} \propto T \end{array} \right.$

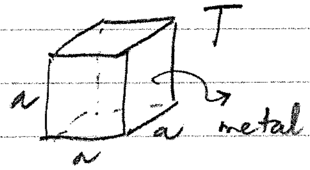
$\Big\} \nearrow$ good @ high freqs onl

- <u>Cavity Radiation</u>

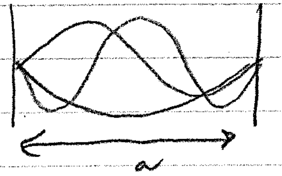


$\boxed{\text{Radiation escaping has Black Body spectrum}}$

Consider cubical cavity



Walls emit a range of frequencies



$\rightarrow \left\{ \begin{array}{l} \text{Wave is } \perp \text{ to wall} \\ \text{Must be } \perp \text{ to } \vec{E} \\ \vec{E}_{\parallel} \text{ must be zero at wall (metal)} \end{array} \right.$

$\rightarrow$ Wave has node at wall

$$\Rightarrow \boxed{\lambda = \frac{2a}{n}} \quad , n = 1, 2, 3$$

So ↳

$$\boxed{E(x,t) = E_0 \sin\left(\frac{2\pi x}{n}\right) \sin\left(2\pi \nu t\right)} \qquad \nu = c/\lambda$$

where $\left\{ \begin{array}{l} E(0,t) = 0 \\ \nu = nc/2a \quad , \quad n = 1, 2, 3 \ldots \end{array} \right. \rightarrow n = 2a\nu/c$

frequencies between ν and $\nu + d\nu$

1-d $\rightarrow$ $N(\nu) d\nu = \frac{2a}{c} d\nu \times 2$ $\rightarrow$ 2 polarizations

Distance in 3-d $\rightarrow$ $r^2 = n_x^2 + n_y^2 + n_z^2$

↳

$$\boxed{\nu = \frac{c}{2a}\sqrt{n_x^2 + n_y^2 + n_z^2}} \qquad n_i \geq 0$$

<u>So</u> $N(r)dr = \frac{1}{8} 4\pi r^2 dr = \frac{\pi r^2}{2} dr$ ↗ first octant   where $r = \frac{2a\nu}{c}$

③

polarizations

$dr = \frac{2a}{c} d\nu$ So $\boxed{N(\nu)d\nu = \frac{\pi}{2}\left(\frac{2a}{c}\right)^3 \nu^2 d\nu \times 2}$

- Energy density $= \boxed{\rho_T(\nu)d\nu = \langle \varepsilon \rangle \frac{N(\nu)d\nu}{a^3}}$

Equipartition theorem ⇒ All modes have avg $KE = \frac{k_BT}{2}$

So $\langle \varepsilon \rangle = k_BT$

So $\boxed{\rho_T(\nu)d\nu = \frac{8\pi \nu^2 k_BT}{c^3} d\nu}$ ⇒ Rayleigh-Jeans formula → only works well at low ν

But problem ⇒ UV catastrophe!

Planck — 1900s

Eq. partition works well here

Rayleigh-Jeans: → $\langle \varepsilon \rangle \xrightarrow[\nu\to 0]{} k_BT$

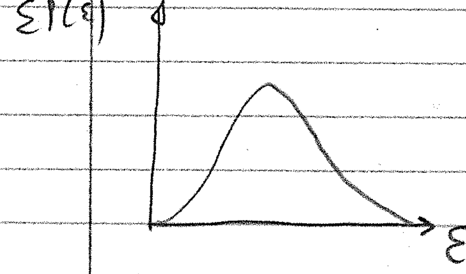
But need $\langle \varepsilon \rangle \xrightarrow[\nu\to\infty]{} 0$

Eq. theorem → $P(\varepsilon) = \frac{1}{kT} e^{-\varepsilon/k_BT}$ → $\langle \varepsilon \rangle = k_BT$

→ ε continuous

Planck says Energy is quantized:

↳ $\langle \varepsilon \rangle = \int \varepsilon P(\varepsilon)d\varepsilon \Big/ \int P(\varepsilon)d\varepsilon$



Do Riemann Sum

- If $\Delta\varepsilon \ll kT$ ⇒ $\langle \varepsilon \rangle = kT$
- If $\Delta\varepsilon \gg kT$ ⇒ $\langle \varepsilon \rangle = 0$

Idea $\boxed{\Delta\varepsilon = h\nu \Rightarrow nh\nu = E \quad , n = 0,1,2,3,}$

Now, $P(\varepsilon) = \frac{1}{kT} e^{-nh\nu/kT}$

So, $$\boxed{\langle\varepsilon\rangle = \frac{\sum^{\infty} \varepsilon P(\varepsilon)}{\sum^{\infty} P(\varepsilon)} = \frac{h\nu}{e^{h\nu/kT}-1}}$$

⟨ε⟩ is frequency dependent.
$$\begin{cases} \langle\varepsilon\rangle \rightarrow k_B T \text{ as } \nu \rightarrow 0 \\ \langle\varepsilon\rangle \rightarrow 0 \text{ as } \nu \rightarrow \infty \end{cases}$$

- Plug this back into $\rho_T(\nu)d\nu = \langle\varepsilon\rangle \frac{N(\nu)d\nu}{a^3}$ & get

$$\boxed{\rho_T(\nu)d\nu = \frac{8\pi\nu^2}{c^3}\left(\frac{h\nu}{e^{h\nu/kT}-1}\right)d\nu}$$

matches Blackbody spectrum very well

→ Energy is Quantized

ep 5, 2019

Waves = Particles

- Classical physics → Waves OR Particles
- Radiation — Photoelectric effect

↳ 1886 - 1887: Hertz discovered γ-electric fx. Problems

① Expect KE of e^- should increase with I of light $\vec{F}_e = e\vec{E}$

→ However, K_{max} of e^- independent of intensity

② If I is high enough, e^- should be ejected regardless of ν

↳ But cutoff ν_0 observed. If $\nu < \nu_0$, no e^- ejected

③ If I is low, it should take time for e^- to be ejected

→ No time delay ever observed.

▨ Einstein: light is packaged in bundles (photons). Usually
(1905) # photons is high enough you see average behavior.

$$E = nh\nu$$

Photoelectric effect: 1 photon with $E = h\nu$ is absorbed by e^- that is then ejected.

$$KE = h\nu - W$$

minimum work to remove e^-

So $\boxed{KE_{max} = h\nu - W_0}$

when $KE_{max} = 0 \rightarrow$ get cutoff ν

↳ Does this fix the problem?

① No I dependence. Only ν

② If $KE = 0$, ν_0 appears naturally. $K = 0 = h\nu_0 - W$

③ Energy deposited by single photons, not spread over surface by wave.

⇒ YES

$\boxed{\text{LIGHT, which is typically a wave, is also a particle}}$

▨ Matter → de Broglie waves (1924)

$$E = h\nu$$

$$\boxed{p = h/\lambda \iff \lambda = h/p} \rightarrow \text{de Broglie relations...}$$

Example e^- scattering in crystal, e^- scatters from atoms + measure angles of the scatter.

⇒ peaks observed that only come from interference

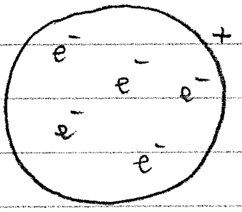
Example Double-slit diffraction with e^-. Same fringe pattern as seen with light.

⇒ Matter (typically particle) is a wave.

—//—

▨ Atomic spectra

⊛ Early 1900's. → J.S. Thomson ⇝ Plum-pudding Model



Knew : # e^- in atom ~ $Z \sim \frac{A}{2}$

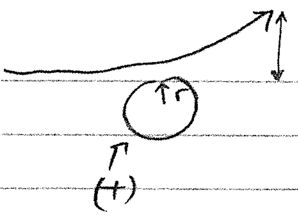
↳ positive charge of Ze to make atoms neutral and massive, as e^- are light

→ But cannot explain atomic spectra.

⊛ 1911 : Rutherford model... Gold foil scattering.

α-particles scatter off gold foil

→ measure scattering angles...



$$\Delta p = F\Delta t = \frac{Q_\alpha Q_n}{r^2} \cdot k(\Delta t)$$

$$= k\,\frac{Q_\alpha Q_n}{r^2}\left(\frac{2r}{V_\alpha}\right)$$

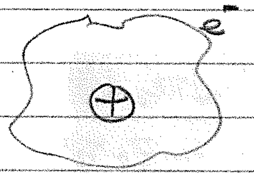
get $\theta = \frac{\Delta p}{p} \simeq 0.0186^\circ \Rightarrow$ plum-pudding doesn't work...

$\searrow$ too small

look at $\Delta p = k\,\frac{Q_\alpha Q_n}{r^2}\left(\frac{2r}{V_\alpha}\right)$

to get $\theta \geq \pi/2$, need $r \simeq 10^{-14}\,m$, not $10^{-10}\,m$ in Thomson model

$\Rightarrow$ Rutherford model...



$r_n \sim 10^{-14}\,m$

$r_{atom} \sim 10^{-10}\,m$

But still not able to explain atomic spectra.

Problem
- If e^- stationary $\Rightarrow$ fall into nucleus by Coulomb
- If e^- orbit $\Rightarrow$ accelerating e^- emitting radiation, and losing energy.

$\rightarrow$ fall into nucleus again

$\Rightarrow$ emitting continuous spectra, NOT discrete

$\boxed{\text{Bohr Model}}$ 4 criteria for e^- behavior:

① e^- move in circular orbits, obey classical mech & Coulomb $\vec{F}$

② e^- can only have orbits with angular momentum of

$$L = n\hbar$$

$$\nu = \frac{|E_f - E_i|}{h}$$

③ e^- emit no radiation, so E_{tot} is constant

④ Radiation is emitted when e^- moves from 1 orbit to another one

discrete
pectra

⇒ mixture of classical + non-classical ...

⇒ accurately describes spectra, but weird...

* * *

Predictions of Bohr Model

Stable orbit: Coulomb force = centripetal force ...

$$\frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r^2} = \frac{mv^2}{r}$$

$$L = n\hbar = mvr \Rightarrow v = \frac{n\hbar}{mr} \quad \text{(quantized)}$$

⇒ Can solve for radius ... $\boxed{r = \frac{4\pi\epsilon_0\hbar^2}{mZe^2n^2} \quad \text{where } n = 1, 2, 3 \ldots}$

Define Bohr radius at $n=1$, $Z=1$

$$\boxed{a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2} \simeq 5.3\times10^{-9}\text{cm} \simeq 0.53\,\text{Å}}$$

$$\boxed{v = \frac{Ze^2}{4\pi\epsilon_0\hbar}\cdot\frac{1}{n}} \quad \text{(quantized)}$$

$$-\frac{Ze^2}{4\pi\epsilon_0 r} = -2KE$$

$$E = KE + PE = \frac{1}{2}mv^2 + PE$$

$$= \frac{Ze^2}{4\pi\epsilon_0(2r)} - \int_r^{+\infty}\frac{Ze^2}{4\pi\epsilon_0 r^2}\,dr$$

<u>So</u> $\boxed{E_n = \frac{-mZ^2e^4}{(4\pi\epsilon_0)^2\,2\hbar^2}\,\frac{1}{n^2}}$ $n = 1, 2, 3, \ldots$ get for $Z=1$ $\boxed{E_1 = -13.6\text{ eV}}$

Sep 6, 2019

Schrödinger Equ

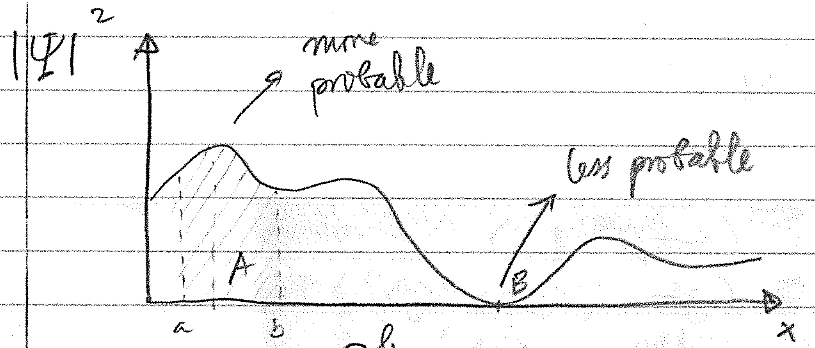
▨ Classical ⟶ $-\frac{\partial V}{\partial x} = m\frac{\partial^2 x}{\partial t^2}$

▨ Quantum ⟶ $i\hbar\,\partial_t \Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$

In the x-direction

$$\hookrightarrow \underbrace{i\hbar\,\partial_t\Psi}_{\text{time evolution}} = \underbrace{-\frac{\hbar^2}{2m}\partial_x^2\Psi}_{p^2/2m} + \underbrace{V\Psi}_{F=-\partial_x V}$$

$p = i\hbar\partial_x$



Ψ : probability amplitude

$|\Psi|^2$: pdf

$$P_{ab} = \int_a^b |\Psi|^2 dx$$

⟨Statistics Review⟩

▨ Discrete Variables

★ Roll die 10 times...

Value (j)	N(j)	P(j)	Δj
1	1	1/10	-2.7
2	2	2/10	-1.7
3	0	0/10	-0.7
4	4	4/10	0.7
5	2	2/10	1.3
6	1	1/10	2.7

- $N = \sum_j N(j) = 10$
- $P(j) = \frac{N(j)}{N}$ $\langle j\rangle = 3.7$
- $\sum_j P(j) = 1$
- Most probable j ⇝ value with highest P(j)
- Mean / Expectation value : $\boxed{\langle j\rangle = \sum_j jP(j}$
- Median j ⇝ 50th quantile (same prob above / below)

More generally ... $\boxed{\langle f(j)\rangle = \sum_j^{\infty} f(j)\, P(j)}$

Ex

$$\langle j^2\rangle = \sum_j^{\infty} j^2 P(j) = 15.9$$

- Spread $\boxed{\Delta j = j - \langle j\rangle}$

- Variance $\sigma^2 = \langle (\Delta j)^2\rangle$

Note $\boxed{\langle j^2\rangle \geq \langle j\rangle^2}$

- Stdev $\sigma = \sqrt{\langle (\Delta j)^2\rangle}$

Now,

$$\begin{aligned}\sigma^2 &= \sum (j - \langle j\rangle)^2 P(j)\\ &= \sum (j^2 - 2j\langle j\rangle + \langle j\rangle^2)\, P(j)\\ &= \langle j^2\rangle - \langle j\rangle^2\end{aligned}$$

So $\boxed{\sigma = \sqrt{\langle j^2\rangle - \langle j\rangle^2}}$

Continuous Variables

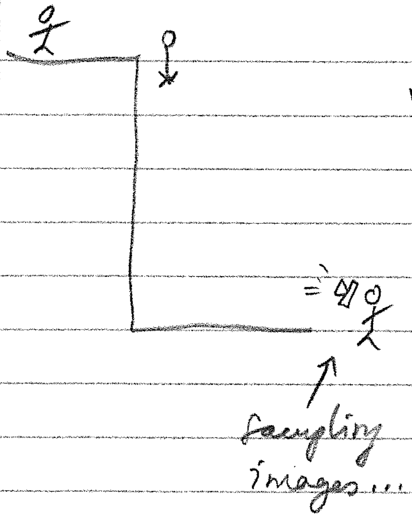
☒ probability density: $p(x)$ (pdf)

and $p(x)dx$ is prob between x & $dx + x$

$$P_{ab} = \int_a^b p(x)\,dx \qquad \langle x\rangle = \int_{-\infty}^{\infty} x\,p(x)\,dx$$

$$1 = \int_{-\infty}^{\infty} p(x)\,dx \qquad \langle f(x)\rangle = \int_{-\infty}^{\infty} f(x)\,p(x)\,dx$$

$$\sigma^2 = \langle x^2\rangle - \langle x\rangle^2$$



What's the average distance travelled?

know $\langle x \rangle < h/2$

$x(t) = \frac{1}{2} g t^2 \quad \frac{dx}{dt} = g t$

$h = \frac{1}{2} g T^2 \Rightarrow T = \sqrt{2h/g}$

Probability of a photo between t & $dt + t$: $\frac{dt}{T} = \frac{dx}{gt} \sqrt{\frac{g}{2h}} = \frac{dx}{2\sqrt{hx}}$

So $p(x) = \begin{cases} \frac{\cancel{dx}}{2\sqrt{hx}} & \text{for } 0 \leq x \leq \cancel{2h}\, h \\ 0 & \text{else.} \end{cases}$

Normalized?

✓

$$\int_{-\infty}^{h} \frac{1}{2\sqrt{hx}} dx = \int_{0}^{h} \frac{1}{2\sqrt{hx}} dx = \frac{1}{2\sqrt{h}} \int_{0}^{h} x^{-1/2} dx = \frac{2\sqrt{h}}{2\sqrt{h}} = 1$$

▨ $\langle x \rangle = \int_{-\infty}^{\infty} x p(x) dx = \int_{0}^{h} x \frac{1}{2\sqrt{hx}} dx = \frac{1}{2\sqrt{h}} \int_{0}^{h} \sqrt{x}\, dx = \frac{2}{3} \frac{1}{2\sqrt{h}} h^{3/2} = \frac{h}{3} < \frac{h}{2}$

▨ For wavefunctions... ——//——

Need ... $\int_{-\infty}^{\infty} |\Psi|^2 dx = 1$

Ψ is a solution to the SE, then $A\Psi$ is also a solution for $A \in \mathbb{C}$

Finding A s.t $\int_{-\infty}^{\infty} |A\Psi|^2 dx = 1$ is called NORMALIZATION.

If there's no such A, then Ψ is probably wrong.
$\rightarrow$ Ψ does not describe a real particle...

☒ But we're only normalizing in x. What abt in t?

Show $$\underbrace{\frac{d}{dt}\int_{-\infty}^{\infty}|\Psi|^2dx}_{\text{fn of t only...}} = 0$$

Pf
$$\frac{d}{dt}\int_{-\infty}^{\infty}|\Psi|^2dx = \int_{-\infty}^{\infty}\frac{\partial}{\partial t}|\Psi|^2dx = \,?$$

Now $$\frac{\partial}{\partial t}|\Psi|^2 = \frac{\partial}{\partial t}\left(\Psi^*\Psi\right) = \left(\frac{\partial}{\partial t}\Psi^*\right)\Psi + \Psi^*\left(\frac{\partial}{\partial t}\Psi\right)$$

Using SE...
$$-i\hbar\,\partial_t\Psi^* = \frac{-\hbar^2}{2m}\partial_x^2\Psi^* + V\Psi^*$$

So $$\frac{\partial}{\partial t}\left(\Psi^*\Psi\right) = \frac{1}{-i\hbar}\left[\frac{-\hbar^2}{2m}\partial_x^2\Psi^* + V\Psi^*\right]\Psi + \Psi^*\frac{1}{i\hbar}\left[\frac{-\hbar^2}{2m}\partial_x^2\Psi + V\Psi\right]$$

$$= \left(\frac{1}{-i\hbar}\,\frac{\hbar^2}{2m}\right)\left[\left(\partial_x^2\Psi^*\right)\Psi - \Psi^*\left(\partial_x^2\Psi\right)\right]$$

$$= \left(\frac{1}{-i\hbar}\,\frac{\hbar^2}{2m}\right)\partial_x\left[\left(\partial_x\Psi^*\right)\Psi - \Psi^*\left(\partial_x\Psi\right)\right]$$

So $$\int_{-\infty}^{\infty}\frac{\partial}{\partial t}|\Psi|^2dx = (\text{stuff})\int_{-\infty}^{\infty}\partial_x\left[\left(\partial_x\Psi^*\right)\Psi - \Psi^*\left(\partial_x\Psi\right)\right]dx$$

$$= (\text{stuff})\left[\left(\partial_x\Psi^*\right)\Psi - \Psi^*\left(\partial_x\Psi\right)\right]\Bigg|_{-\infty}^{\infty} = 0 \quad \text{since} \begin{cases}\Psi\rightarrow 0 \text{ at } \infty\\ \partial_x\Psi\rightarrow 0 \text{ at } \infty\end{cases}$$

Sep 9, 2019

Momentum

$$\langle x\rangle = \int_{-\infty}^{\infty} x\,|\Psi(x,t)|^2\,dx$$. How does this evolve?

$$\frac{d}{dt}\langle x\rangle = \frac{d}{dt}\int_{-\infty}^{\infty} x\,|\Psi(x,t)|^2\,dx = \int_{-\infty}^{\infty} x\,\partial_t|\Psi|^2\,dx$$

$$= \int_{-\infty}^{\infty} x\left[(\partial_t\Psi^*)\Psi + \Psi^*(\partial_t\Psi)\right]dx$$

(SE)

▨ Can find, using SE

$$\frac{d}{dt}\langle x\rangle = \frac{i\hbar}{2m}\int_{-\infty}^{\infty} x\,\partial_x\left(\Psi^*(\partial_x\Psi) - (\partial_x\Psi^*)\Psi\right)dx$$

▨ Now, integration by parts...

$$\int_{-\infty}^{\infty} x\,\partial_x\left[\Psi^*(\partial_x\Psi) - (\partial_x\Psi^*)\Psi\right]dx$$

$$= \underbrace{x\left[\Psi^*(\partial_x\Psi) - (\partial_x\Psi^*)\Psi\right]\Bigg|_{-\infty}^{\infty}}_{0} - \int_{-\infty}^{\infty}\left[\Psi^*(\partial_x\Psi) - (\partial_x\Psi^*)\Psi\right]dx$$

$$= 0 - \underbrace{\int_{-\infty}^{\infty}\left[\Psi^*(\partial_x\Psi) - (\partial_x\Psi^*)\Psi\right]}dx$$

Integration by parts again...

$$\int_{-\infty}^{\infty}\Psi(\partial_x\Psi^*)dx = \underbrace{\Psi^*\Psi\Big|_{-\infty}^{\infty}}_{0} - \underbrace{\int_{-\infty}^{\infty}(\partial_x\Psi)\Psi^*dx}$$

So $$\frac{d}{dt}\langle x\rangle = \frac{i\hbar}{2m}\cdot\left[-2\int_{-\infty}^{\infty}(\partial_x\Psi)\Psi^*dx\right]$$

~~So,~~ $\cancel{\boxed{\frac{d}{dt}\langle x\rangle = 0}}$ So, $$\boxed{\frac{d}{dt}\langle x\rangle = \frac{-i\hbar}{m}\int_{-\infty}^{\infty}\Psi^*(\partial_x\Psi)dx}$$

▨ In general, we work with momentum, so,

$$\boxed{\langle p\rangle \overset{?}{=} m\frac{d\langle x\rangle}{dt} = -i\hbar\int_{-\infty}^{\infty}\Psi^*(\partial_x\Psi)\,dx}$$

▨ Call momentum an operator → $\hat{p}$.

$$\langle x\rangle = \int_{-\infty}^{\infty}\Psi^*\, x\, \Psi\, dx$$

→ order is now important.

$$\langle p\rangle = \int_{-\infty}^{\infty}\Psi^*\underbrace{(-i\hbar)\,\partial_x}_{\hat{p}}\Psi\, dx$$

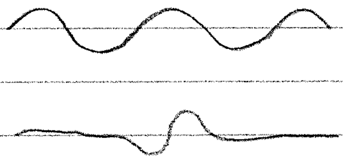
▨ $\hat{T} = \frac{1}{2}mv^2 = \frac{\hat{p}^2}{2m}$; $\hat{\vec{L}} = \hat{r}\times\hat{p}$

▨ In general, for any operator Q

$$\boxed{\langle Q(x,p)\rangle = \int_{-\infty}^{\infty}\Psi^*(Q(x,p))\,\Psi\, dx}$$

//

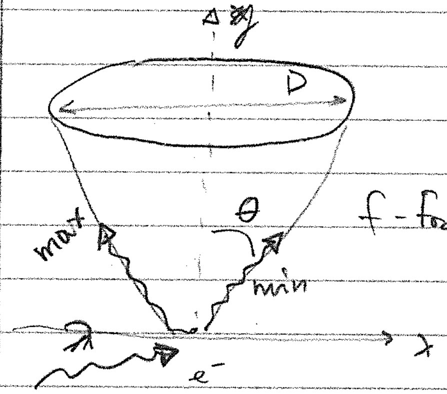
UNCERTAINTY PRINCIPLE



Trade off between position & wavelength, i.e, between position and momentum.

▨ Heisenberg uncertainty principle $\boxed{\sigma_x \sigma_p \geq \frac{\hbar}{2}}$

▨ Heisenberg Microscope



Momentum has to conserve

	Before	After
min	$p = \frac{h}{\lambda} + 0$	$\frac{h}{\lambda'}\sin\theta + mv_x'$
max	$p = \frac{h}{\lambda} + 0$	$\frac{-h}{\lambda''}\sin\theta + mv_x''$

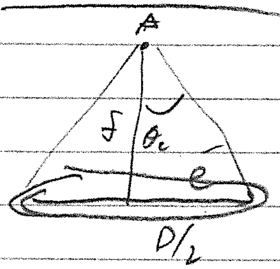
- So, electron momentum is either

$$mv_x' = \frac{h}{\lambda} - \frac{h}{\lambda'}\sin\theta \quad \text{or} \quad mv_x'' = \frac{h}{\lambda} + \frac{h}{\lambda''}\sin\theta$$

- For $\theta \ll 1$, then $\sin\theta \sim \theta$ and $\lambda \sim \lambda' \sim \lambda''$, so

$$\Delta p \sim \frac{2h}{\lambda}\theta$$ ⇒ If λ small, then Δp big

What about Δx?



$\sin\theta_c \simeq \frac{\lambda}{D}$. For small angle, $\theta_c \sim \frac{\lambda}{D}$

So position can be resolved between

$$\begin{array}{ccc} -f\sin\theta_c & \text{and} & +f\sin\theta_c \\ \wr & & \wr \\ -f\frac{\lambda}{D} & \text{and} & f\frac{\lambda}{D} \end{array}$$

So, $\lambda\downarrow \Rightarrow \Delta x\downarrow$

But $\frac{f}{D} = \frac{1}{2\tan\theta} \sim \frac{1}{2\theta}$ so, $\boxed{\Delta x = \frac{\lambda}{2\theta} - \left(-\frac{\lambda}{2\theta}\right) = \frac{\lambda}{\theta}}$

- $$\Delta x \Delta p \cong \frac{\lambda}{\theta} \cdot \frac{2h}{\lambda}\cancel{\theta} \sim 2h > \frac{\hbar}{2}$$

—#—

ep 11, 2019

$\boxed{\text{STATIONARY STATES + SEPERATION OF VARS}}$

SE

$$i\hbar\, \partial_t \Psi = \frac{-\hbar^2}{2m} \partial_x^2 \Psi + V\Psi$$

In general, $V = V(x,t)$. But most of what we do $V = V(x)$

$$\Psi = \psi(x)\, \varphi(t)$$

Then $i\hbar\, \partial_t \Psi = i\hbar\, \psi\, d_t \varphi(t)$; $\partial_x^2 \Psi = \varphi(t)\, \partial_x^2 \psi$

Then $(i\hbar\, \partial_t \varphi)\psi = \frac{-\hbar^2}{2m} \varphi\, \partial_x^2 \psi + V\psi\varphi$

$$\text{So} \quad \underbrace{(i\hbar) \frac{\partial_t \varphi}{\varphi}}_{\text{time only}} = \underbrace{\frac{-\hbar^2}{2m} \frac{\partial_x^2 \psi}{\psi} + V}_{\text{space only}} = \text{Constant}$$

Define separation constant as E. Write

$$\boxed{i\hbar \frac{\partial_t \varphi}{\varphi} = E} \quad \text{and} \quad \boxed{\frac{-\hbar^2}{2m} \frac{\partial_x^2 \psi}{\psi} + V = E}$$

time - independent SE

Solution

$$\boxed{\varphi(t) = e^{-iEt/\hbar}}$$

▨ Why are separable solutions good?

(1) They are stationary states $\Psi = \psi e^{-iEt/\hbar}$

$$\rightarrow |\Psi|^2 = \psi^*\psi \, e^{-iEt/\hbar} e^{iEt/\hbar} = |\psi|^2$$

→ time dependence cancels out (only true if E real)

In fact,

$$\boxed{\langle Q(x,p)\rangle = \int_{-\infty}^{\infty} \psi^* \left[Q(x, -i\hbar\partial_x) \right] \psi \, dx}$$

→ No time dependence when calc. exp values

(2) They have definite energies

Total energy = KE + PE ⇝ Hamiltonian...

$$H = \frac{p^2}{2m} + V$$

as operators...

$$\boxed{\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}} \quad \text{or} \quad \boxed{\hat{H} = \frac{-\hbar^2}{2m}\partial_x^2 + \hat{V}}$$

or one write $\hat{H}\psi = E\psi$

and so

$$\langle H\rangle = \int \psi^* \underset{\sim}{\hat{H}\psi} \, dx = \int E \psi^*\psi \, dx = E$$

$$\langle H^2\rangle = \ldots = E^2$$

So $\boxed{\sigma_H = 0}$ → No uncertainty in E

→ Total energy is always E.

(3) General solution is a linear combination of separable sols

Time ind SE has infinitely many solutions $\psi_1, \psi_2, \ldots$ for $E_1, E_2, E_3, \ldots$

$$\Psi_n(x,t) = \psi_n \varphi_n$$

$$\Psi_n(x,t) = \psi_n e^{-iE_n t/\hbar}$$

General solution: $$\boxed{\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n \exp\left[-iE_n t/\hbar\right]}$$

Pf Let $\Psi(x,t) = \sum_{n=1}^{\infty} c_n \Psi_n$

Then $$i\hbar\, \partial_t \Psi = i\hbar\, \partial_t \left(\sum c_n \Psi_n \right)$$

$$= \sum c_n \left(i\hbar\, \partial_n \Psi_n \right)$$

$$= \sum c_n \left[\frac{-\hbar^2}{2m} \partial_x^2 \Psi_n + V \Psi_n \right]$$

$$= \frac{-\hbar^2}{2m} \partial_x^2 \Big(\underbrace{\sum c_n \Psi_n}_{\Psi} \Big) + V \Big(\underbrace{\sum c_n \Psi_n}_{\Psi} \Big) \qquad \square$$

* * *

Strategy for finding $\Psi(x,t)$

① Solve time-ind SE for given $V(x)$ → find ψ_n, E_n

② Find c_n from $\Psi(x,0) = \sum c_n \psi_n$

③ Add time dependence ⇒ get $\Psi(x,t) = \sum c_n \psi_n \exp(-iE_n t/\hbar)$

Note Ψ_n is a stationary state. Ψ is not.

Ex Let $\Psi = c_1\Psi_1 + c_2\Psi_2 = c_1\psi_1 e^{-iE_1t/\hbar} + c_2\psi_2 e^{-iE_2t/\hbar}$

$$|\Psi|^2 = \underbrace{c_1^*c_1|\Psi_1|^2 + c_2^*c_2|\Psi_2|^2}_{\text{no time dep}} + \underbrace{c_1c_2^*\Psi_1\Psi_2^* + c_1^*c_2\Psi_1^*\Psi_2}_{\text{time-dependence}}$$

So $\boxed{\Psi \text{ is not a stationary state}}$

⟹ Interpret $|c_n|^2$ as the probability a measurement would yield E_n

$$\sum |c_n|^2 = 1$$

and so $\boxed{\langle H\rangle = \sum |c_n|^2 E_n}$ → independent of time
→ Conservation of Energy

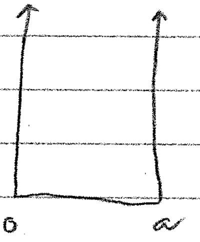
$\langle H\rangle$ not always an allowed E_n

But a measurement always gives allowed E_n.

Sep 12, 2019

Infinite Square Well

$$V(x) = \begin{cases} 0 & 0 \le x \le a \\ \infty & \text{otherwise} \end{cases}$$



Outside well → $\psi = 0$

Inside well → $-\frac{\hbar^2}{2m}\partial_x^2\psi_{in} + \cancelto{0}{0\psi} = E\psi_{in}$

So $\boxed{\partial_x^2\psi_{in} = -k^2\psi_{in}}$ where $k = \sqrt{\frac{2mE}{\hbar}}$ ← assuming E positive

Is $E>0$?

$\frac{-\hbar^2}{2m}\partial_x^2\psi + V\psi = E\psi \Rightarrow \partial_x^2\psi = \frac{2m}{\hbar}(V-E)\psi$. If $E<V \Rightarrow V-E>0$

$$\rightarrow \partial_x^2\psi = \overset{\nearrow\ \text{positive}}{a}\psi \Rightarrow \boxed{\text{blow up}}\ \text{positive} \Leftrightarrow \text{need cutoff.}$$

- If $E > V$, then $\partial_x^2\psi = -a\psi \rightsquigarrow$ good.

$$\boxed{\partial_x^2\psi_{in} = -k\psi_{in}} \Rightarrow \text{general solution } \boxed{\psi_{in}(x) = A\sin(kx) + B\cos(kx)}$$

→ find A, B from boundary condition...

$$\boxed{\begin{Bmatrix} \text{(1) } \psi \text{ continuous} \\ \text{(2) } \partial_x\psi \text{ continuous except where } V = \infty \end{Bmatrix}}$$

Integrate SE from $-\varepsilon$ to ε, then take limit as $\varepsilon \to 0$

$$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{\varepsilon}\partial_x^2\psi\,dx + \int_{-\varepsilon}^{\varepsilon}V\psi\,dx = \underbrace{\int_{-\varepsilon}^{\varepsilon}E\psi\,dx}_{0}$$

$$-\frac{\hbar^2}{2m}\partial_x\psi\Big|_{-\varepsilon}^{\varepsilon}$$

. Now, take the limit...

▨ $$\Delta(\partial_x\psi) = \lim_{\varepsilon\to 0}\left(\partial_x\psi\Big|_{\varepsilon} - \partial_x\psi\Big|_{-\varepsilon}\right) = \frac{2m}{\hbar}\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon}V\psi\,dx = 0$$

except where $V = \infty$

$\Rightarrow \partial_x\psi$ continuous.

We need $\psi(0) = \psi(a) = 0 \Rightarrow \boxed{B = 0,\ k = \frac{\pi n}{a}}$

So $$\boxed{\psi(x) = A\sin\left(\frac{\pi n}{a}x\right)}$$

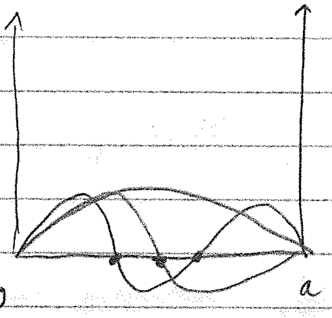
quantized

Now $$k = \frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{a} \Rightarrow \boxed{E_n = \frac{\hbar^2 n^2\pi^2}{2ma^2},\ n = 1, 2, 3, \dots}$$

Find A by normalizing wfn ⇒ $1 = \int_0^a A^2 \sin^2\left(\frac{\pi n}{a} x\right) dx$

$$= A^2 \cdot \left(\frac{a}{2}\right) \rightarrow \boxed{A = \sqrt{\frac{2}{a}}}$$

So $\boxed{\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right)}$



Properties

true for symmetric V(x)

① Alternate even & odd with respect to center of wells

true ∀ V(x)

② Each higher energy gets an extra node. (# nodes = n−1)

③ Wavefunctions are mutually orthogonal } → true in general...

orthonormality

(always true)

$$\int_{-\infty}^{\infty} \psi_m^* \psi_n \, dx = \frac{2}{a}\int_{-\infty}^{\infty} \sin\left(\frac{\pi n}{a} x\right) \sin\left(\frac{\pi m}{a} x\right) dx$$

$$= \frac{1}{a}\int_0^a \cos\left(\frac{m-n}{a} x\pi\right) - \cos\left(\frac{m+n}{a} x\pi\right) dx$$

$$= \boxed{0} \quad \text{if } m \neq n$$

So $\boxed{\int_{-\infty}^{\infty} \psi_m^* \psi_n \, dx = \delta_{mn}}$

④ Completeness : any other function can be written as a linear combination of these.

(always true)

$$\boxed{\psi(x) = \sum_{n=1}^{\infty} c_n \psi_n = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{a} x\right)}$$

Fourier series. Any periodic fn can be written as a sum of sines/cosines

To find c_n, use orthonormality.

$$\int \psi_m^* \Psi\, dx = \int \psi_m^* \sum c_n \psi_n\, dx = \int \delta_{mn}\, c_n \psi_m^* \psi_n\, dx$$

$$= c_m$$

Thus $$\boxed{c_m = \int_{-\infty}^{\infty} \psi_m^* \psi\, dx}$$

☒ So, stationary states...

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)\cdot e^{-iE_n t/\hbar} = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)\exp\left[\frac{-in^2\hbar^2\pi^2 t}{\hbar}\right]$$

☒ The general solution is

$$\boxed{\Psi(x,t) = \sum_{n=1}^{\infty} \Psi_n c_n = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}}\sin\left(\frac{\pi n}{a}x\right)\exp\left[\frac{-in^2\hbar^2\pi^2 t}{\hbar}\right]}$$

To find c_n, look at $\Psi(x,0) = \sum c_n \psi_n$

well then $$c_n = \sqrt{\frac{2}{a}}\int_0^a \sqrt{\frac{a}{2}}\,\psi_n^*\,\Psi(x,0)\, dx$$

$$c_n = \sqrt{\frac{2}{a}}\int_0^a \sin\left(\frac{n\pi}{a}x\right)\cdot\Psi(x,0)\, dx \quad \ldots$$

Normalization check

$$1 = \int |\Psi(x,0)|^2 dx = \int \sum^{\infty} c_n^* \Psi_n^* \cdot \sum^{\infty} c_m \Psi_m\, dx$$

$$= \sum_{m,n} (c_m^* c_m)(\delta_{mn})$$

$$= \sum |c_m|^2 = 1 \quad ✓$$

Expectation value of Hamiltonian?

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

$$\hat{H}\psi_n = E_n\psi_n$$

So $$\langle H\rangle = \int \psi^* \hat{H}\psi \, dx = \int\left(\sum c_n^* \psi_n^*\right)\left(\sum_m c_m E_m \psi_m\right) dx$$

$$= \sum_{m,n} c_n^* c_m E_m \int \psi_n^* \psi_m \, dx$$

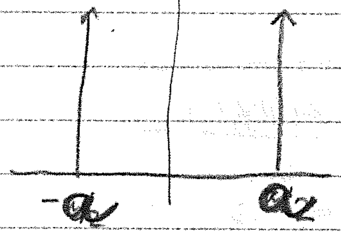
$$= \sum_{m,n} c_n^* c_m E_m \delta_{mn}$$

$$\boxed{\langle H\rangle = \sum_n |c_n|^2 E_n}$$

Sep 13, 2019

//

Suppose we have a new potential $V(x) = \begin{cases} 0 & -a \leq x \leq a \\ \infty & \text{else} \end{cases}$



well $\psi = A\cos(kx) + B\sin(kx)$

$$\psi(a) = \psi(-a) = 0$$

$$\psi(a) = A\sin(ka) + B\cos ka = 0$$
$$\psi(-a) = -A\sin(ka) + B\cos ka = 0$$

So $\psi(a) + \psi(-a) = 2B\cos(ka) = 0 \Rightarrow k = \left(j - \frac{1}{2}\right)\frac{\pi}{a}$

$\psi(a) - \psi(-a) = 2A\sin(ka) = 0 \Rightarrow k = \frac{j\pi}{a}$

▨ If $B = 0$, $A \neq 0$, then $k = \frac{j\pi}{a}$. But notice that the ground state, centered at the middle, cannot be a sin() (because $\sin(x) = 0$ @ $x = 0$)

$\Rightarrow$ Let $n = 2j$, $k = \frac{n\pi}{2a}$

$$\Rightarrow \psi_{even} = A\sin\left(\frac{\pi n}{2a}x\right)$$

Normalize ⇒ $1 = |A|^2 \int_{-a}^{a} \sin^2\left(\frac{n\pi}{2a}x\right) dx \Rightarrow \boxed{A = \frac{1}{\sqrt{a}}}$

▨ Let $A = 0,\ B \neq 0$, $k = \left(j - \frac{1}{2}\right)\frac{\pi}{a}$. Let $n = 2j - 1 \Rightarrow k = \frac{n\pi}{2a}$

$\psi_{odd} = B\cos\left(\frac{n\pi}{2a}x\right)$. Normalize… $\boxed{B = \frac{1}{\sqrt{a}}}$

$$k = \sqrt{\frac{2mE}{\hbar^2}} = \frac{n\pi}{2a} \Rightarrow \boxed{E = \frac{n^2\hbar^2\pi^2}{2m(2a)^2}}$$

So

$\psi_n = \frac{1}{\sqrt{a}}\left(\sin\left(\frac{n\pi}{2a}x\right)\right)$ if n is even

$\psi_n = \frac{1}{\sqrt{a}}\left(\cos\left(\frac{n\pi}{2a}x\right)\right)$ if n is odd

But we could have gotten the same thing letting $x \to \left(\frac{x+a}{2}\right)$

//

SIMPLE HARMONIC OSCILLATOR

▨ Classical → mass on spring $F = -kx = \frac{dp}{dt} = m\frac{d^2x}{dt^2}$

General soln: $x(t) = A\cos(\omega t) + B\sin(\omega t)$

$\omega = \sqrt{k/m}$

$$V = -\int F dx = \frac{1}{2}kx^2$$

▨ $V(x) \sim V(x_0) + V'(x_0)(x - x_0) + \frac{V''(x_0)}{2}(x - x_0)^2 + \ldots$

So $V(x) \sim \frac{1}{2}V''(x_0)(x - x_0)^2 \ldots \Rightarrow$ most potentials can be approximated locally like this…

▨ Quantum $\boxed{V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2}$

So SE: $\frac{-\hbar^2}{2m}\partial_x^2\Psi + \frac{1}{2}m\omega^2x^2\Psi = i\hbar\,\partial_t\Psi$

Time-ind $-\frac{\hbar^2}{2m}\partial_x^2\psi + \frac{1}{2}m\omega^2x^2\psi = E\psi$

Define dimensionless variable ... $\xi = \sqrt{\frac{m\omega}{\hbar}}\,x$

Then $\partial_x = \frac{d\xi}{dx}\partial_\xi$, $\partial_x^2 = \left(\frac{d\xi}{dx}\right)^2\partial_\xi^2$

⇒ new SE:

$$\frac{-\hbar^2}{2m}\left(\frac{m\omega}{\hbar}\right)\partial_\xi^2\psi + \frac{1}{2}m\omega^2\frac{\hbar}{m\omega}\xi^2\psi = E\psi$$

So $\partial_\xi^2\psi = \left(\frac{m\omega}{\hbar}x^2 - \frac{2E}{\hbar\omega}\right)\psi$

So $\boxed{\partial_\xi^2\psi = (\xi^2 - k)\psi}$ $k = 2E/\hbar\omega$

▨ For $\xi \gg k$ ⇒ $\partial_\xi^2\psi = \xi^2\psi$

$$\psi(\xi) = Ae^{-\xi^2/2} + Be^{\xi^2/2}$$

Since $\psi(\xi)$ has to be normalizable, $B = 0$

So at large ξ (large x), $\boxed{\psi(\xi) = Ae^{-\xi^2/2}}$

↑ this is probably a polynomial

So $\boxed{\psi(\xi) = h(\xi)e^{-\xi^2/2}}$

↳ Now, plug back into the SE. Find derivs first...

☒ $$\frac{d\psi}{d\xi} = \left(h'(\xi) - \xi h(\xi)\right) \exp\left[-\xi^2/2\right]$$

☒ $$\frac{d^2\psi}{d\xi^2} = \left(h''(\xi) - 2\xi h'(\xi) + (\xi^2 - 1) h(\xi)\right) \exp\left[-\xi^2/2\right]$$

$\Rightarrow$ Put back into SE : $\partial_\xi^2 \psi = (\xi^2 - k)\psi$ to get

$$\boxed{\partial_\xi^2 h - 2\xi \frac{dh}{d\xi} + (k-1) h(\xi) = 0}$$

Suppose $h(\xi)$ is a polynomial, then $h(\xi) = \sum_{j=0}^{\infty} a_j \xi^j$

So $$h'(\xi) = \sum_{j=0}^{\infty} j a_{j+1} \xi^{j-1}$$

$$h''(\xi) = \sum_{j=0}^{\infty} (j+1)(j+2) a_{j+2} \xi^{j}$$

Sep 16, 2019 **So** back to SE

$$\sum_{j=0}^{\infty} (j+1)(j+2) a_{j+2} \xi^{j} - 2\xi \sum_{j=0}^{\infty} j a_{j+1} \xi^{j-1} + (k-1) \sum_{j=0}^{\infty} a_j \xi^j = 0$$

$$\sum_{j=0}^{\infty} (j+1)(j+2) a_{j+2} \xi^{j} - 2j a_{j+1} \xi^j + (k-1) a_j \xi^j = 0$$

$$\Leftrightarrow \quad (j+1)(j+2) a_{j+2} \xi^{j} - 2j a_{j+1} \xi^j + (k-1) a_j \xi^j = 0$$

$$\Leftrightarrow \quad (j+1)(j+2) a_{j+2} - 2j a_{j+1} + (k-1) a_j = 0$$

$$\Leftrightarrow \quad \boxed{a_{j+2} = \frac{(2j - k + 1)}{(j+1)(j+2)} a_j}$$

if a_0 known $\Rightarrow$ a_{2n} known
a_1 known $\Rightarrow$ a_{2n+1} known

And so we can rewrite $h(\xi)$ as

$$h(\xi) = (a_0 + a_2\xi^2 + a_4\xi^4 + \ldots) + (a_1\xi + a_3\xi^3 + \ldots)$$

So $h(\xi) = h_{even}(\xi) + h_{odd}(\xi)$

Next, need h to be normalizable. At large j, $a_{j+2} \sim \frac{2}{j} a_j$

and $a_j \sim \frac{c}{(j/2)!}$. Then

$$h(\xi) = c \sum_j \frac{1}{(j/2)!} \xi^j = c \sum 1/j! \, \xi^{2j} \quad \text{(not normalizable)}$$

$$\Rightarrow \boxed{h(\xi) \simeq C \exp[\xi^2]} \quad \text{for large } j.$$

↓ still problematic ⇒ need to truncate series at some j.

⇒ need $a_{j+2} = 0$ when $j =$ some n

↳ this means either the even or odd must be zero.

So $a_0 = 0$ if n odd
$a_1 = 0$ if n even

We have $2j - k + 1 = 0$ when $j = n \Rightarrow k = 2n + 1$

$$k = \frac{2E}{\hbar\omega} \Rightarrow \boxed{E_n = \left(n + \frac{1}{2}\right)\hbar\omega}$$ for allowed energies for SHO
$n = 0, 1, 2, \ldots$

Put this back... $$\boxed{a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)} a_j}$$

If $n = 0$, then $j = 0$ ⇒ get only a_0. $h(\xi) = a_0$

If $n = 1$, then $a_0 = 0$..., get only a_1 $h(\xi) = a_1 \xi^1$

If $n = 2$, then a_0, a_2 $h(\xi) = a_0 + a_2 \xi^2$

Now, $\psi(\xi) = h(\xi) \exp\left[-\xi^2/2\right]$

so $\psi_0(\xi) = a_0 \exp\left[-\xi^2/2\right]$ $\qquad$ $\psi_2(\xi) = (a_0 + a_2\xi^2) \exp\left[\xi^2/2\right]$

$\psi_1(\xi) = a_1 \xi \exp\left[-\xi^2/2\right]$ $\qquad\qquad \vdots$

→ h is polynomial of degree n

If n is even, then get only even ~~numbers~~ powers.

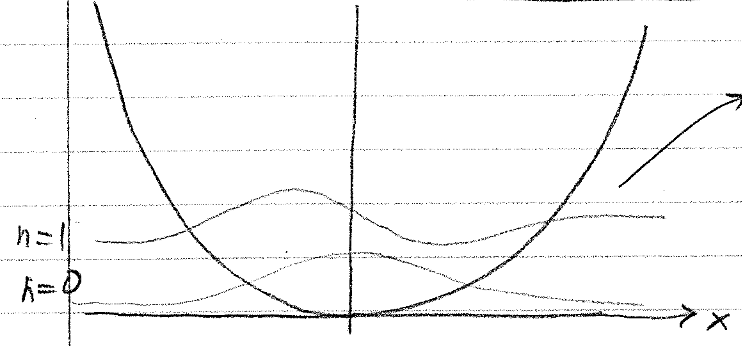
If n is odd, - - only odd powers.

☒ $h(\xi)$ are Hermite polynomials $H(\xi)$, apart from factor of a_0 (or) a_1 ...

☒ By convention, the highest power of ξ has coef 2^n. Then normalize.

After normalizing,

$$\boxed{\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}}$$



there's non-zero probability of finding particle outside the potential.

↳ This was not possible w/ ∞ V

☒ For odd states, the probability of particle at center is 0

For infinite square well, # nodes = 1

For SHO, # nodes = n

—//—

$\boxed{\text{SHO: Ladder Operators}}$

SE: $$-\frac{\hbar^2}{2m}\partial_x \Psi + \frac{1}{2}m\omega^2 x^2 \Psi = E\Psi$$

☒ Rewrite in terms of operators:

$$\underbrace{\frac{1}{2m}\left[\hat{p}^2 + (m\omega\hat{x})^2\right]}_{\hat{H}} \Psi = E\Psi \longrightarrow \text{need to factor } \hat{H}!$$

$$\hat{x}\hat{p}\, f(x) = x(-i\hbar\partial_x f)$$
$$\hat{p}\hat{x}\, f(x) = (-i\hbar)\,\partial_x(xf) = -i\hbar f - i\hbar x\partial_x f$$

$$\boxed{[\hat{x}\hat{p} - \hat{p}\hat{x}]f = i\hbar f}$$

$\uparrow$

Commutator: $[\hat{x},\hat{p}] = i\hbar$

Next, define $$\boxed{\hat{a}_\pm = \frac{1}{\sqrt{2\hbar m\omega}}\left(\mp i\hat{p} + m\omega\hat{x}\right)}$$ → ladder operators...

ep 18, 2019

Then

$$\hat{a}_-\hat{a}_+ = \frac{1}{2\hbar m\omega}\left(i\hat{p} + m\omega\hat{x}\right)\left(-i\hat{p} + m\omega\hat{x}\right)$$

$$\boxed{\hat{a}_-\hat{a}_+ = \frac{1}{2\hbar m\omega}\left(\hat{p}^2 + (m\omega\hat{x})^2 - im\omega[\hat{x},\hat{p}]\right)}$$

So $$\hat{a}_-\hat{a}_+ = \frac{\hat{H}}{\hbar\omega} + \frac{i}{2\hbar}\overbrace{[\hat{x},\hat{p}]}^{i\hbar} = \frac{\hat{H}}{2\hbar} + \frac{1}{2}$$

So $\hat{a}_-\hat{a}_+ = \frac{\hat{H}}{\hbar\omega} + \frac{1}{2} \rightarrow$ $\boxed{\begin{aligned}\hat{H} &= \left(\hat{a}_-\hat{a}_+ - \frac{1}{2}\right)\hbar\omega \\ &= \left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)\hbar\omega\end{aligned}}$

If we let $\hat{a}_- = \hat{a}$, $\hat{a}_+ = \hat{a}_-^+ = \hat{a}^+$ then $\hat{H} = \left(\hat{a}^+\hat{a} + \frac{1}{2}\right)\hbar\omega$

Another thing ...

$$\boxed{[\hat{a}_-, \hat{a}_+] = 1}$$

Can write SE in terms of these ... $\hat{H}\Psi = E\Psi$. So

$$(\hbar\omega)\left(\hat{a}_-\hat{a}_+ - \frac{1}{2}\right)\Psi = E\Psi = \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)\Psi$$

If Ψ is a solution then so is $\hat{a}_+\Psi$. If has energy E, $\hat{a}_+\Psi$ has energy $E + \hbar\omega$.

$$\begin{aligned}
\hat{H}(\hat{a}_+\Psi) &= \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)\hat{a}_+\Psi \\
&= \hbar\omega\left[\hat{a}_+\hat{a}_-\hat{a}_+\Psi + \frac{1}{2}\hat{a}_+\Psi\right] \\
&= \hbar\omega\,\hat{a}_+\left[\hat{a}_-\hat{a}_+ + \frac{1}{2}\right]\Psi \\
&= \hat{a}_+\left\{\hbar\omega\left(\hat{a}_-\hat{a}_+ - \frac{1}{2}\right) + \hbar\omega\right\}\Psi \\
&= \hat{a}_+\left(\hat{H} + \hbar\omega\right)\Psi \\
&= \hat{a}_+\left(E + \hbar\omega\right)\Psi
\end{aligned}$$

So $\boxed{\hat{H}(\hat{a}_+\Psi) = (E + \hbar\omega)\hat{a}_+\Psi}$

Similarly, $\boxed{\hat{H}\hat{a}_-\psi = (E-\hbar\omega)\hat{a}_-\psi}$

$$\begin{cases} \hat{a}_+ \text{ moves up energy states} \rightarrow \text{Raising operator} \\ \hat{a}_- \text{ moves down energy} \rightarrow \text{Lowering operator} \end{cases}$$

If ψ_n is known, all ψ_n can be found.

Need to avoid $E<0 \Rightarrow \boxed{\hat{a}_-\psi_0 = 0}$

Recall $\hat{a}_- = \frac{1}{\sqrt{2\hbar m\omega}}\left(+i\hat{p} + m\omega\hat{x}\right)\psi_0 = 0$

$$\Rightarrow \frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\partial_x + m\omega\hat{x}\right)\psi_0 = 0$$

$$\Rightarrow \partial_x\psi_0 = \frac{-m\omega}{\hbar}x\psi_0$$

$$\Rightarrow \boxed{\psi_0 = \left(\sqrt{\frac{m\omega}{\hbar\pi}}\right)^{1/4}\exp\left[\frac{-m\omega x^2}{2\hbar}\right]}$$ ⇝ after normalization.

Energy $\hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)\psi_0 = E_0\psi_0$

$$\Rightarrow \frac{1}{2}\hbar\omega\psi_0 = E_0\psi_0 \Rightarrow \boxed{E_0 = \frac{1}{2}\hbar\omega}$$

and so $\boxed{E_n = \hbar\omega\left(n+\frac{1}{2}\right)}$

→ Also note: $\boxed{\hat{a}_+\hat{a}_-\psi_n = n\psi_n}$

Find Ψ_1 ... $\Psi_1 = A_1 (\hat{a}_+)^1 \Psi_0$

$$= A_1 \frac{1}{\sqrt{2m\hbar\omega}} \left(-i\hat{p} + m\omega\hat{x}\right) \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left\{\frac{-m\omega x^2}{2\hbar}\right\}$$

$$= A_1 \frac{1}{\sqrt{2\hbar m\omega}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \left(\cancel{\hbar} m\omega x + m\omega x\right) \exp\left\{\frac{-m\omega x^2}{2\hbar}\right\}$$

$$= A_1 \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{\frac{m\omega}{2\hbar}}\, x \exp\left\{\frac{-m\omega x^2}{2\hbar}\right\}$$

turns out $A_1 = 1$

$$\rightarrow \Psi_1 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \sqrt{\frac{m\omega}{2\hbar}}\, x \exp\left\{\frac{-m\omega x^2}{2\hbar}\right\}, \quad E_1 = \frac{3}{2}\hbar\omega$$

* * *

☒ Now, recall that

$$\Psi_n = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H(\xi) \exp\left[-\xi^2/2\right] \; ; \; \xi = \sqrt{\frac{m\omega}{\hbar}}\, x$$

$H_0 = 1, \quad H_1 = 2\xi, \ldots$

→ everything matches, which is nice!

☒ Next, how to find A_n without normalizing?

↳ use ladder operators...

SHO ladder operator

Sep 19, 2019

$\psi_n(x) = A_n(\hat{a}_+)^n \psi_0 \quad n = 0, 1, 2, \ldots \quad E_n = (n+\frac{1}{2})\hbar\omega$

Normalize $\quad \hat{a}_+\psi_n = c_n\psi_{n+1}, \quad \hat{a}_-\psi_n = d_n\psi_{n-1}$

$$\int_{-\infty}^{\infty} f^*(\hat{a}_\pm g)\,dx = \int_{-\infty}^{\infty}(\hat{a}_\mp f)^* g\,dx$$

or $\longrightarrow$ $\langle f|\hat{a}_\pm g\rangle = \langle \hat{a}_\mp f|g\rangle$

$\hat{a}_+$ and $\hat{a}_-$ are adjoints / hermitian conjugates...

So...
$$\int_{-\infty}^{\infty}(\hat{a}_\pm\psi_n)^*(\hat{a}_\pm\psi_n)\,dx = \int_{-\infty}^{\infty}\hat{a}_\mp\hat{a}_\pm\psi_n$$

$$\int_{-\infty}^{\infty}(\hat{a}_+\psi_n)^*(\hat{a}_+\psi_n)\,dx = |c_n|^2\int|\psi_{n+1}|^2 dx = |c_n|^2$$

Recall $\quad \hat{a}_-\hat{a}_+\psi_n = (n+1)\psi_n$

$\hat{a}_+\hat{a}_-\psi_n = n\psi_n$

So $\displaystyle\int_{-\infty}^{\infty}(n+1)\psi_n^*\psi_n\,dx = |c_n|^2 \Rightarrow \boxed{c_n = \sqrt{n+1}}$

and $\displaystyle\int_{-\infty}^{\infty} n\,\psi_n^*\psi_n\,dx = |d_n|^2 \Rightarrow \boxed{d_n = \sqrt{n}}$

$$\boxed{\begin{aligned}\hat{a}_+\psi_n &= \sqrt{n+1}\,\psi_{n+1}\\ \hat{a}_-\psi_n &= \sqrt{n}\,\psi_{n-1}\end{aligned}}$$

$$\rightarrow \boxed{\begin{aligned} \psi_{n+1} &= \frac{1}{\sqrt{n+1}}\,\hat{a}_+\psi_n \\ \psi_{n-1} &= \frac{1}{\sqrt{n}}\,\hat{a}_-\psi_n \end{aligned}}$$

$$\boxed{\psi_n = \frac{1}{\sqrt{n!}}\left(\hat{a}_+\right)^n\psi_0} \quad \text{where } \psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left[\frac{-m\omega x^2}{2\hbar}\right]$$

Note all these ψ_n's are orthonormal...

$$\boxed{\int_{-\infty}^{\infty}\psi_m^*\left(\hat{a}_+\hat{a}_-\right)\psi_n\,dx = \int_{-\infty}^{\infty}\psi_m^*\, n\,\psi_n\,dx = n\,\delta_{mn}}$$

Lastly, writing $\hat{x}$ & $\hat{p}$ in terms of $\hat{a}_+, \hat{a}_-$

$$\boxed{\begin{aligned} \hat{x} &= \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}_+ + \hat{a}_-\right) \\ \hat{p} &= i\sqrt{\frac{\hbar m\omega}{2}}\left(\hat{a}_+ - \hat{a}_-\right) \end{aligned}}$$

* * *

Sep 20, 2019

$\boxed{\text{Free Particle}}$ $V(x) = 0$

Time Indep. SE $\rightsquigarrow$ $\dfrac{-\hbar^2}{2m}\partial_x^2\psi + 0 = E\psi$

so $\boxed{\partial_x^2\psi = -k^2\psi}$ $k = \sqrt{\dfrac{2mE}{\hbar^2}}$

no quantization of E so long as E > 0

Solution (no boundaries...): $\boxed{\psi = Ae^{+ikx} + Be^{-ikx}}$

moving to the right

moving to the left

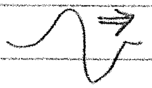
Add in time dependence... $\exp\left[-iEt/\hbar\right]$ -

$$\text{So} \quad \boxed{\Psi = A\exp\left[ik\left(x - \frac{\hbar k}{2m}t\right)\right] + B\exp\left[-ik\left(x + \frac{\hbar k}{2m}t\right)\right]}$$

Can also write $\Psi = A\cos(kx \pm vt) + iB\sin(kx \pm vt)$

Nodes at $kx \pm vt = \left(n + \frac{1}{2}\right)\pi$

$$\hookrightarrow \quad x = \left(n + \frac{1}{2}\right)\frac{\pi}{k} \pm \frac{vt}{k}$$



⇒ Traveling wave ⇒ As t increases, all nodes go together

$\left\{\begin{array}{l} A \text{ term} \Rightarrow \text{wave moving right} \\ B \text{ term} \Rightarrow \text{wave moving left} \end{array}\right\}$ same energies...

$$\boxed{\Psi_k = A\exp\left[i\left(kx - \frac{\hbar k^2}{2m}t\right)\right] \quad ; \quad k = \pm\sqrt{2mE}/\hbar}$$

If $k > 0$ ⇒ going right ; $k < 0$ ⇒ going left

de Broglie ⇝ $\lambda = \frac{2\pi}{|k|}$; $p = \hbar k$.

Speed of wave...

$$V_{\text{quantum}} = \frac{\text{coef of } t}{\text{coef of } x} = \frac{\hbar |k|}{2m}.$$

However... $V_{\text{classical}} = \; --- \; = \frac{\hbar|k|}{2m}$.

☒ Now, note that we can't normalize Ψ_k ...

$$\int_{-\infty}^{\infty} |\Psi_k|^2 \, dx = |A|^2 \int_{-\infty}^{\infty} \exp\left[-i\left(kx - \frac{\hbar k^2}{2m}\right)\right] \exp\left[+i\left(kx - \frac{\hbar k^2}{2m}\right)\right] dx$$

$$= |A|^2 \int_{-\infty}^{\infty} dx \rightarrow \text{doesn't converge!}$$

↳ No stationary states ⇒ No states w/ definite energy.

→ Ψ_k is not a physical solution, but a linear combo can be.

→ Consider general solution... → ~~take Fourier transform of $\phi(k)$~~

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) \exp\left[i\left(kx - \frac{\hbar k^2}{2m} t\right)\right] dk}$$

⇓

where $\frac{1}{\sqrt{2\pi}} \phi_k(k)\, dk \rightsquigarrow$ wave packet

↳ play the role of c_n

$\Psi(x,t)$ contains a range of energy + speed → wave packet.

Consider $$\boxed{\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) \exp\left[+ikx\right] dk}$$

Fourier transform...

inverse ⇝ $$f(x) = \mathcal{F}\left[F(k)\right](x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{ikx} \, dk$$

forward ⇝ $$F(k) = \mathcal{F}^{-1}\left[f(x)\right](k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} \, dx$$

With this, can find $\phi(k)$...

To find $\phi(k)$...

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0)\, e^{-ikx}\, dx$$

$\boxed{\text{Ex}}$ <u>Problem 2.20</u>:

$$\Psi(x,0) = A \exp\left[-a|x|\right]$$

First, normalize... $1 = \int |\Psi(x,0)|^2 dx = |A|^2 \int_{-\infty}^{\infty} \exp\left[-2a|x|\right] dx$

$$= 2|A|^2 \underbrace{\int_0^{\infty} \exp\left[-2ax\right] dx}_{1/2a}$$

$$\rightarrow A = \sqrt{a}$$

Now, take FT to find $\phi(k)$...

$$\phi(k) = \mathcal{F}\left[\Psi(x,0)\right](k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0)\, e^{-ikx}\, dx$$

$$= \sqrt{\frac{a}{2\pi}} \int_{-\infty}^{\infty} \exp\left[-\cancel{2}a|x|\right] e^{-ikx}\, dx$$

0

$$= \sqrt{\frac{a}{2\pi}} \int_{-\infty}^{\infty} \exp\left[-a|x|\right] \left(\cos kx - i \sin kx\right) dx$$

$\frac{1}{2}\left(e^{-ikx} + e^{+ikx}\right)$

$$= 2\sqrt{\frac{a}{2\pi}} \int_0^{\infty} \exp\left[-a|x| \cancel{-ikx}\right] dx$$

$$= 2\sqrt{\frac{a}{2\pi}} \int_0^{\infty} \exp\left[-ax \cancel{-ikx}\right] dx$$

<u>So</u> $\phi(k) = \sqrt{\frac{a}{2\pi}} \int_0^{\infty} \exp\left(x(ik-a)\right) + \exp\left(-x(ik+a)\right) dx$

$$= \sqrt{\frac{a}{2\pi}} \left[\frac{\exp\left[(ik-a)x\right]}{(ik-a)} + \frac{\exp\left[-(ik+a)x\right]}{-(ik+a)} \right] \Bigg|_0^{\infty}$$

At ∞, we get cancellation. At 0, we can combine terms...

$$\boxed{\phi(k) = \sqrt{\frac{a}{2\pi}}\left(\frac{2a}{k^2+a^2}\right)}$$

So now,

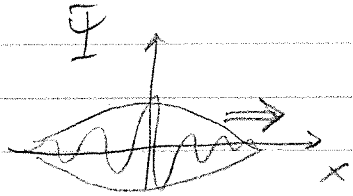
$$\boxed{\Psi(x,t) = \frac{a^{3/2}}{\pi}\int_{-\infty}^{\infty}\frac{1}{k^2+a^2}\exp\left[i\left(kx-\frac{\hbar k^2}{2m}t\right)\right]dk}$$

ep 23, 2011

Speed of wave ... $v = \frac{\text{coef of } t}{\text{coef of } x} = \sqrt{\frac{E}{2m}} = \frac{1}{2}v_{\text{classical}}$

Why not $v_{\text{classical}}$? ⇒ Because this is a wave packet,

i.e. the velocity is group velocity.



Shape: amplitude determined by combination of $\phi(x)$.

2 velocities ⇒ group velocity (of envelope)
speed to ripple (phase velocity)

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int\phi(k)\exp\left[i(kx-\omega t)\right]dk$$

For us $\omega = \frac{\hbar k^2}{2m}$ ⇝ dispersion relation

$$\omega(k) \simeq \omega_0 + \underbrace{(k-k_0)}_{s}\omega_0' + \dots \qquad \omega_0' = \left.\frac{d\omega}{dk}\right|_{k=k_0}$$

With this,

$$\boxed{\Psi(x,t) \simeq \frac{1}{\sqrt{2\pi}}\int\phi(k_0+s)\exp\Big[i\big((k_0+s)x-(\omega_0+\omega_0's)t\Big]ds}$$

$$\simeq \underbrace{\frac{1}{\sqrt{2\pi}} \exp\left[i(k_0 x - \omega_0 t)\right]}_{\text{ripples}} \cdot \underbrace{\int \phi(k_0+s) \exp\left[is(x-\omega_0' t)\right]}_{\text{envelope}} ds$$

So $\boxed{v_{phase} = \frac{\omega_0}{k_0}, \quad v_{group} = \omega_0'}$

In general, $\boxed{v_{phase} = \frac{\omega}{k} ; \quad v_{group} = \frac{d\omega}{dk}}$

With $\omega = \frac{\hbar k^2}{2m}$, $\quad v_{phase} = \frac{\hbar k}{2m} = \frac{p}{2m} = \sqrt{\frac{E}{2m}}$

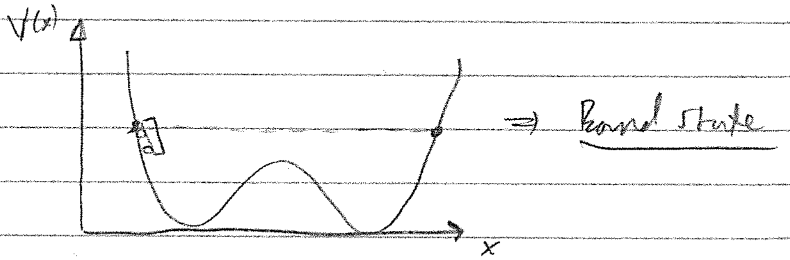
$$v_{group} = \frac{d\omega}{dk} = \frac{\hbar k}{m} = \sqrt{\frac{2E}{m}} \rightsquigarrow v_{classical}$$

↳ group velocity is classical, but phase velocity different.

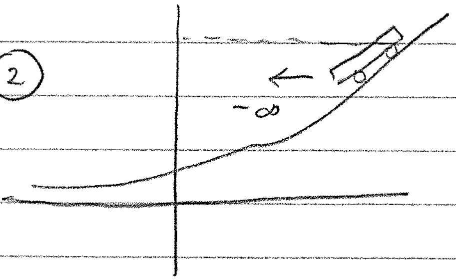
BOUND vs SCATTERING STATES

Classical cart on hill...

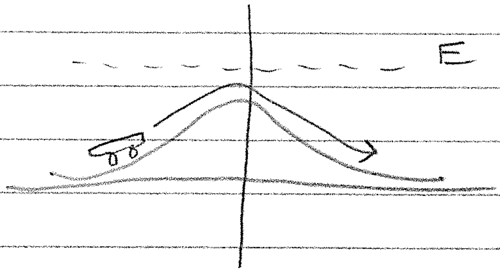
①



②

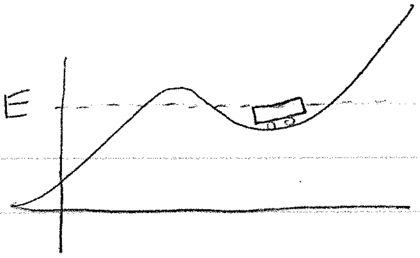


③



Scattering states

QM

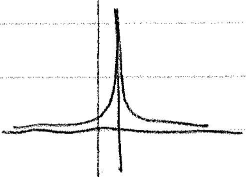


classically bounded
but QM, particle can tunnel thru
→ QM only bounded when $E < V(\infty)$

In reality, $V(\pm\infty) \to 0$, so $\begin{cases} E<0 & \text{bound} \\ E>0 & \text{scattering} \end{cases}$

There are potentials of both kinds...

DELTA FUNCTION WELL



$$\delta(x) = \begin{cases} 0 & \text{if } x \neq 0 \\ \infty & \text{if } x = 0 \end{cases} \qquad \int \delta(x)\,dx = 1$$

In general... $\delta(x-a) = \begin{cases} 0 & \text{if } x \neq a \\ \infty & \text{if } x = a \end{cases}$

$$\int_{-\infty}^{\infty} f(x)\,\delta(x-a)\,dx = f(a)$$

Let potential $V(x) = -\alpha\,\delta(x)$

$$\boxed{\frac{-\hbar^2}{2m}\partial_x^2 \psi - \alpha\,\delta(x)\,\psi = E\psi}$$

Bound state $E<0$

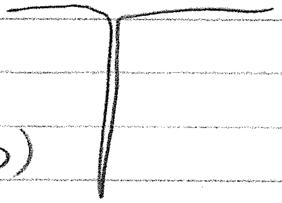
Look at $x<0$ then $x>0$, then use continuity conditions to connec

$x<0$ $\quad \frac{-\hbar^2}{2m}\partial_x^2\psi = E\psi \quad , \quad k = \sqrt{\frac{-2mE}{\hbar}}$

$$\partial_x^2\psi = k^2\psi$$

$$\psi(x) = Ae^{+kx} + \cancel{Be^{-kx}} \to 0 \text{ (unphysical)} \quad \to \quad \psi(x) = \cancel{B}e^{+kx}$$

$x > 0, \quad \psi(x) = Ce^{-kx} + \cancel{De^{+kx}}$ → unphysical



So $$\psi(x) = \begin{cases} Be^{kx} & x < 0 \\ Ce^{-kx} & x \geq 0 \end{cases} \qquad (E<0)$$

Continuity condition ⇒ $\psi(x)$ cont everywhere
⇒ @ $x=0$, $B=C$

$\frac{d\psi}{dx}$ must be continuous everywhere unless there is an ∞ boundary...

ep 25, 2019

Recall ... (9/12)

$$\Delta \partial_x \psi = \lim_{\varepsilon\to 0}\left(\partial_x\psi\Big|_{+\varepsilon} - \partial_x\psi\Big|_{-\varepsilon}\right) = \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon} V(x)\psi(x)\,dx$$

$-\alpha\delta(x)$

$$\Rightarrow \Delta\partial_x\psi = \left(-\frac{2m\alpha}{\hbar^2}\right)\psi(0).$$

Thus $-\cancel{B}k\exp[kx]\Big|_{x=0} - \cancel{B}k\exp[-kx]\Big|_{x=0} = \frac{-2m\alpha}{\hbar^2}\cancel{B}$

So $$k = \frac{2m\alpha}{2\hbar^2} = \frac{m\alpha}{\hbar^2} = \frac{\sqrt{-2mE}}{\hbar}$$

$$\Rightarrow \boxed{E = \frac{-m\alpha^2}{2\hbar^2}}$$ ⤳ Energy of bound state.

Normalize to find B...

$$1 = \int_{-\infty}^{\infty}|\psi(x)|^2 dx = 2|B|^2\int_0^{\infty}\exp[-2kx]\,dx \rightsquigarrow 1 = \frac{|B|^2}{k} \Rightarrow \boxed{B = \frac{\sqrt{m\alpha}}{\hbar}}$$

For bound states... $(E<0)$
only one bound state ⟹ $$\boxed{\psi(x) = \frac{\sqrt{m\alpha}}{\hbar}\exp\left[\frac{-m\alpha|x|}{\hbar^2}\right], \quad E = \frac{-m\alpha^2}{2\hbar^2}}$$

$\boxed{E>0}$ ⇝ scattering states... $\partial_x^2 \psi = \frac{-2mE}{\hbar^2}\psi = -k^2\psi$

⇝ free particle. $k = \frac{\sqrt{2mE}}{\hbar}$

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & (x<0) \\ Fe^{ikx} + Ge^{-ikx} & (x>0) \end{cases}$$

① ψ continuous $\Rightarrow$ $A+B = F+G$

② $\partial_x \psi$ continuous except @ ∞ boundaries... Integrate SE

$$ik\left(Fe^{ikx} - Ge^{-ikx}\right) - ik\left(Ae^{ikx} - Be^{-ikx}\right) = \frac{-2m\alpha}{\hbar^2}\underbrace{(A+B)}_{\psi(0)}$$

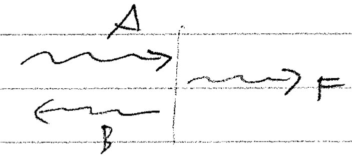
$$\text{At } x=0 \Rightarrow ik\left[F-G-A+B\right] = -\frac{2m\alpha}{\hbar^2}(A+B)$$

$$\Rightarrow (F-G) = A(1+2i\beta) - B(1-2i\beta) \text{ w/ } \boxed{\beta = \frac{m\alpha}{\hbar^2 k}}$$

Put in the time dependence... For both $x<0$ & $x>0$, have wave traveling left + wave traveling right.

$x<0$ ⇝ A right, B left

$x>0$ → F right, G left



Imagine wave coming from $x=-\infty$. Then we don't want anything coming from the left @ $x>0$ ⇒ $G=0$.

A: incident; B= reflected $x=-\infty$, F transmitted $+\infty$

Relative Probability ⇝ Reflection: $\boxed{R = \frac{|B|^2}{|A|^2}}$

↳ Transmission: $\boxed{T = \frac{|F|^2}{|A|^2}}$

In reality, we want the relative {flux = velocity × intensity}

So $R = \frac{v_r |B|^2}{v_i |A|^2} = \frac{|B|^2}{|A|^2}$ because velocities are the same

$T = \frac{v_t |F|^2}{v_i |A|^2} = \frac{|F|^2}{|A|^2}$ because velocities are the same

- Next, write F, B in terms of A...

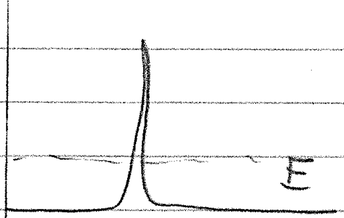
$$\boxed{F = \frac{1}{1-i\beta} A} \qquad \boxed{B = \frac{i\beta}{1-i\beta} A}$$

So $\boxed{R = \frac{\beta^2}{1+\beta^2}, \quad T = \frac{1}{1+\beta^2}}$ Notice $\boxed{R + T = 1}$

$$\beta = \frac{m\alpha}{\hbar^2 k} \rightsquigarrow \boxed{\begin{aligned} R &= \frac{m\alpha/\hbar^2 k}{1+\left(\frac{m\alpha}{\hbar^2 k}\right)^2} = \frac{1}{1+\left(2\hbar^2 E/m\alpha^2\right)} \\ T &= \;\dots\; = \frac{1}{1+\left(m\alpha^2/2\hbar^2 E\right)} \end{aligned}}$$

[!] What if we have δ fn barrier, $V(x) = +\alpha\delta(x)$

↳ Everything same except sign of α. But there are no bound states because $V(x) = 0$ everywhere...



⇝ Still get T, R even though there's an infinite barrier.

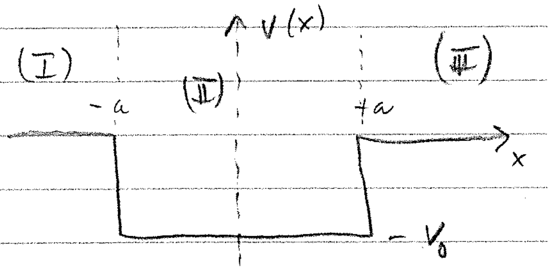
↳ Tunneling

Ψ as we wrote it is not normalizable (free particle eigenstate)
→ need combo of Ψ_k.

⇒ R & T are approximates for waves with energy around $\underline{E}$.

ep 26, 2019

FINITE SQUARE WELL



$$V(x) = \begin{cases} -V_0 & -a \leq x \leq a \\ 0 & |x| > a \end{cases}$$

Bound states: $(E < 0)$

(I) $x < -a$ $\quad \partial_x^2 \Psi = k^2 \Psi$ $\qquad k = \frac{\sqrt{-2mE}}{\hbar}$

(II) $|x| \leq a$ $\quad \partial_x^2 \Psi = -l^2 \Psi$

(III) $x > a$ $\quad \partial_x^2 \Psi = k^2 \Psi$ $\qquad l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$

$$\Psi(x) = \begin{cases} \cancelto{0}{Ae^{-kx}} + Be^{kx} & x < -a \\ C\sin(lx) + D\cos(lx) & -a \leq x \leq a \\ Fe^{-kx} + \cancelto{0}{Ge^{kx}} & x > a \end{cases}$$

A, G = 0 to keep Ψ normalizable. From infinite square well we know we need alternating even + odd solutions

Even solutions ⇝ only cosine term in the well...

$\Psi(x) = \Psi(-x)$ ⇒ $B = F$ to be symmetric.
Since symmetric, look at $x = a$, need look at $x = -a$.

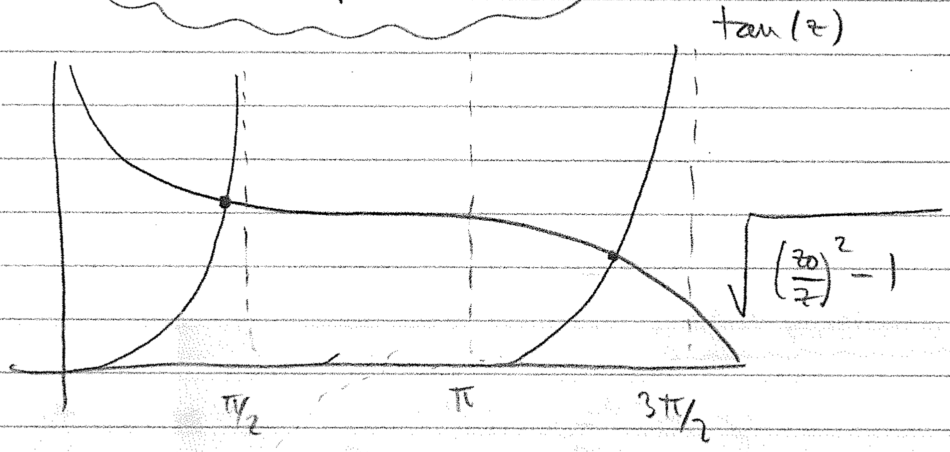
$$\left.\begin{array}{ll} \Psi \text{ continuous} \Rightarrow & Fe^{-ka} = D\cos(la) \quad @\ x = a \\ \partial_x \Psi \text{ continuous} \Rightarrow & -kFe^{-ka} = -lD\sin(la) \end{array}\right\}$$

So $\boxed{k = l\tan(la)}$ ⤳ this is an equation for E.

Let $z = la$, $z_0 = \frac{a}{\hbar}\sqrt{2mV_0}$

↑ includes E ↑ width + depth of well...

So, $$\tan(z) = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$$



① Looking at limiting cases...

(a) Wide + deep well ... z_0 large. Intercept with z axis moves right $\sqrt{(z_0/z)^2 - 1}$ moves up.

↳ Intersection gets closer to $z_n = \frac{n\pi}{2}$ $(n = 1, 3, 5 \ldots, \ldots 5)$

So $z_n = \frac{\sqrt{2m(E_n + V_0)}}{\hbar} a \cong \frac{n\pi}{2} \Rightarrow \boxed{E_n \simeq \frac{n^2\pi^2\hbar^2}{2m(2a)^2} - V_0}$

like ∞ square well...

↳ $n = 1, 3, 5, \ldots$

⇒ This is half of ∞ square well states with bottom of well @ $-V_0$, width $2a$.

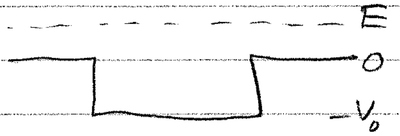
(b) Shallow + narrow : z_0 small

Intercept moves closer to $z = 0$

If $z < \pi/2 \Rightarrow$ have only one intersection

$\rightarrow$ only 1 bound states $\Rightarrow$ at least one bound state regardless of how small the well is.

$\boxed{\text{Odd states}}$ $\rightsquigarrow$ Exercise ...



E > 0 Scattering states

$$k = \frac{\sqrt{2mE}}{\hbar} \qquad l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$$

Then

$$\psi(x) = \begin{cases} Ae^{+ikx} + Be^{-ikx} & x < -a \\ C\sin(lx) + D\cos(lx) & -a < x < a \\ Fe^{ikx} + \underset{\swarrow\,0}{Ge^{-ikx}} & a < x \end{cases}$$

Nothing coming from $x > a \Rightarrow G = 0$.

$$x = -a \Rightarrow \begin{cases} Ae^{-ika} + Be^{ika} = -C\sin(la) + D\cos(la) \\ ik(Ae^{-ika} + Be^{ika}) = +Cl\cos(la) - Dl\sin(la) \end{cases}$$

$$x = +a \Rightarrow \begin{cases} Fe^{ika} = +C\sin(la) + D\cos(la) \\ ikFe^{ika} = +Cl\cos(la) - Dl\sin(la) \end{cases}$$

5 unknowns...

$$B = i\frac{\sin(2la)}{2kl}(l^2-k^2)F \quad ; \quad F = \frac{\exp[-2ika]}{\cos(2la) - i\frac{k^2+l^2}{2kl}\sin(2la)}A$$

$$\boxed{T = \frac{|F|^2}{|A|^2} = \left(1 + \frac{V_0^2}{4E(E+V_0)} \sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)\right)^{-1}}$$

If $T = 1$, then $\sin^2(\ldots) = 0 \Leftrightarrow$ ~~$E+V_0 = n\pi \Leftrightarrow E_n = \pi n - V_0$~~

$$\Leftrightarrow \frac{2a}{\hbar}\sqrt{2m(E+V_1)} \Leftrightarrow \boxed{E_n = \frac{n^2\pi^2\hbar^2}{2m(2a)^2} - V_0}$$

↑ infinite square well...

ep 27, 2019

Review

① General approach to solving potentials... ⇝ split into regions...
② Write SE for each region
③ Write general s/n
④ Apply boundary conditions + continuity conditions

- ψ cont everywhere
- $\partial_x\psi$ cont except @ ∞ boundary

$$\Delta\partial_x\psi = \frac{2m}{\hbar^2}\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon} V(x)\psi(x)\,dx$$

- ψ go to 0 @ ∞
- For symmetric potential, alternate even ~ odd between center of well...

⑤ Find allowed energies...
⑥ Normalize or find R or T

Ladder operators (QSHO)

$$\hat{a}_\pm = \frac{1}{\sqrt{2\hbar m\omega}}\left[\mp i\hat{p} + m\omega\hat{x}\right] \rightsquigarrow \begin{cases} \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}_+ + \hat{a}_-\right) \\ \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}\left(\hat{a}_+ - \hat{a}_-\right) \end{cases}$$

$\hat{a}_+ \psi_n = \sqrt{n+1}\, \psi_{n+1}$; $\hat{a}_- \psi_n = \sqrt{n}\, \psi_{n-1}$; $\hat{a}_- \psi_0 = 0$

$\langle \hat{Q} \rangle = \int \Psi^* \hat{Q} \Psi dx$

Bound state: $E < V$ @ $\pm\infty$ Most $V \to 0$ @ $\pm\infty$ so

Scattering state $E > V$ @ $\pm\infty$

$\begin{cases} E < 0 & \text{bound} \\ E > 0 & \text{scattering} \end{cases}$ (most)

But $E > V_{min}$ always...

---

ep 30, 2019

$\boxed{\text{Even \& odd Wfn}}$ (Bound states only)

$$-\frac{\hbar^2}{2m} \partial_x^2 \psi + V\psi = E\psi$$

Let $V(x)$ be symmetric (even) $\rightsquigarrow V(x) = V(-x)$

Let $x \to -x$

$$-\frac{\hbar^2}{2m} \partial_x^2 \psi(-x) + V(-x)\psi(-x) = E\psi(-x)$$

$$-\frac{\hbar^2}{2m} \partial_x^2 \psi(-x) + V(x)\psi(-x) = E\psi(-x)$$

So $\psi(x)$ solves $\Longrightarrow$ $\psi(-x)$ solves with energy E.

Write solution as lin. comb of these...

$$\psi_{even} \propto \psi(x) + \psi(-x)$$

$$\psi_{odd} \propto \psi(x) - \psi(-x)$$

For 1D potentials can't have degenerate solutions

$\hookrightarrow \psi(x) = c\psi(-x) \rightsquigarrow c = \pm 1 \rightsquigarrow \psi(x) = \pm \psi(-x)$

$\psi(-x) = c^2 \psi(x)$ $\to$ even or odd only

HILBERT SPACE - BRAKET NOTATION

Wfns represent state of system and are abstract vectors

Operators act on wfn are matrices ...

(1) (ket) $|\alpha\rangle \rightsquigarrow a = (a_1 \ldots a_N)^T$

(2) (bra) $\langle\alpha| \rightsquigarrow a = (a_1^* \ldots a_N^*)$

(3) $$\langle\alpha|\alpha\rangle = \sum_{i=1}^{N} a_i^* a_i$$

(4) $$\langle\beta|\alpha\rangle = \sum_{i=1}^{N} b_i^* a_i$$

$$\hat{T}|\alpha\rangle = Ta = \begin{pmatrix} T_{11} & \cdots & T_{1N} \\ \vdots & & \\ T_{N1} & \cdots & T_{NN} \end{pmatrix} \begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix} = \ldots$$

All wfn of x form a vector space. }
Want normalizability }

$\Rightarrow$ want square-integrable $\int_a^b |f(x)|^2 dx < \infty$

$\Rightarrow$ wfns that do this form a Hilbert space.

$$\boxed{\langle f|g\rangle = \int f^* g}$$

$$\boxed{\langle g|f\rangle = \int g^* f}$$

$$\langle f|g\rangle = \langle g|f\rangle^*$$

$$\langle f|f\rangle = \int |f|^2 dx$$

$$\langle f_m|f_n\rangle = \delta_{mn}$$

$$f(x) = \sum c_n f_n \rightarrow c_n = \langle f_n|f\rangle$$

Oct 3, 2019

OBSERVABLES

$$\langle \hat{Q} \rangle = \int \Psi^* Q \Psi \, dx = \langle \Psi | \hat{Q} \Psi \rangle \rightsquigarrow \text{real, } \cancel{\text{force}} \ \underbrace{\hat{Q} = \hat{Q}^\dagger}_{\text{Hermitian}}$$

$$\langle \hat{a} \rangle^* = \int (Q^\dagger \Psi)^* \Psi \, dx = \langle \hat{Q}^\dagger \Psi | \Psi \rangle = \langle \hat{Q} \Psi | \Psi \rangle$$

$$\rightarrow \boxed{\text{For } \hat{Q} = \hat{Q}^\dagger, \ \langle \Psi | \hat{Q} \Psi \rangle = \langle \hat{Q} \Psi | \Psi \rangle}$$

Ex $$\langle f | \hat{p} g \rangle = \int f^* (-i\hbar \partial_x) g = -i\hbar f^* g \Big|_{-\infty}^{\infty} + \int_{-\infty}^{\infty} (-i\hbar \partial_x f)^* g \, dx$$

$$= \langle \hat{p} f | g \rangle$$

☒ If we prepare a state that gives q every time you measure it is a determinate state.

Ex Stationary states are determinate states of $\hat{H}$

$$\boxed{\sigma_q^2 = 0} = \langle \hat{Q}^2 \rangle - \langle Q \rangle^2$$

$$= \langle (Q - \langle Q \rangle)^2 \rangle$$

$$= \langle \Psi | (Q - \langle Q \rangle)^2 \Psi \rangle$$

$$= \langle \underbrace{(Q - \langle Q \rangle)\Psi}_{0} | \underbrace{(Q - \langle Q \rangle)\Psi}_{0} \rangle = 0$$

→ **Eigenfunctions of operators**

$\hat{Q}\Psi = q\Psi \rightarrow q$ is a number. Collection of q form a spectrum

- Eigenfunctions w/ the same eigenvalue are degenerate.

Discrete Spectra

Thm 1 : Eigenvalues of Hermitian Operators are real

$$\hat{Q}f = qf \qquad \langle f|\hat{Q}f\rangle = \langle f|qf\rangle = q\langle f|f\rangle$$

$$\langle \hat{Q}f|f\rangle = \langle q^{*}f|f\rangle = q^{*}\langle f|f\rangle \qquad \rightarrow q = q^{*}$$

Thm 2 : If eigenfunctions to Hermitian have different eigenvalues, they are orthogonal

$$\hat{Q}f = qf, \quad \hat{Q}g = q'g \qquad \langle f|\hat{Q}g\rangle = \langle \hat{Q}f|g\rangle$$

$$q'\langle f|g\rangle = q\langle f|g\rangle$$

Since $q' \neq q \Rightarrow \langle f|g\rangle = 0$

Axiom Eigenfunctions of an observable are complete

This can be proven for a finite vector space and some special infinite case ...

Continuous Spectra

→ Eigenfunctions not normalizable
→ not vectors in Hilbert space ...

But we want $\langle f_n|f_m\rangle = \delta_{mn}$ (Kronecker delta)

→ for continuous case $\boxed{\langle f_n|f_{n'}\rangle = \delta(n'-n)}$ → Dirac delta

Say, f_p is an eigenfn of $\hat{p}$ w/ eigenvalue p.

$$\rightarrow \boxed{\hat{p}f_p = pf_p = -i\hbar\partial_x f_p}$$

Solve this to get $f_p(x) = A\exp\left[ipx/\hbar\right]$

If $p \in \mathbb{C}\setminus\mathbb{R} \Rightarrow$ not normalizable.

If $p \in \mathbb{R} \Rightarrow$ good, normalizable ...

$$\delta(p'-p) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i(p'-p)x/\hbar}\,dx$$

$$\int_{-\infty}^{\infty} f_{p'}^*(x)\, f_p(x)\,dx = |A|^2 \underbrace{\int_{-\infty}^{\infty} \exp\left[i(p-p')x/\hbar\right]dx} \longrightarrow \sim \delta(p-p')\,(2\pi\hbar)$$

$$= |A|^2(2\pi\hbar)\,\delta(p-p') \,.\ \text{If } A = 1/\sqrt{2\pi\hbar} \text{ then}$$

$$\int_{-\infty}^{\infty} f_{p'}^*(x) f_p(x) = \boxed{\delta(p-p') = \langle f_{p'} | f_p \rangle}$$

So we get $\langle f_{p'} | f \rangle = \displaystyle\int_{-\infty}^{\infty} c(p)\, \langle f_{p'} | f_p \rangle\, dp$

$$= \int_{-\infty}^{\infty} c(p)\,\delta(p-p')\,dp = c(p')$$

$$\Rightarrow \boxed{f(x) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} c(p)\exp\left[ipx/\hbar\right]dp = \mathcal{F}\left[c(p)\right](x)}$$

Oct 4, 2019

STATISTICAL INTERPRETATION

☒ If you measure observable $\hat{Q}(x,y) \Rightarrow$ get eigenvalue ...

☒ If spectrum discrete, probability of getting q_n is $\boxed{P(q_n) = \left|\langle f_n | \Psi \rangle\right|^2 = |c_n|}$

☒ If spectrum cont., get a range dz $\boxed{P(dz) = |c(z)|^2 dz}$

☑ When performing measurement, wfn collapse to the eigenstate or a range around the eigenstate for continuous...

☑ Conceptually, $\Psi(x,t) = \sum c_n(t)\psi_n(x)$

$$c_n(t) = \langle \psi_n | \Psi \rangle = \int \psi_n^* \Psi \, dx$$

↳ c_n is how much of n^{th} state is inside Ψ, measurement probability $= |c_n|^2$.

$$\boxed{\begin{aligned} 1 = \sum |c_n|^2 = \sum |\langle \psi_n | \Psi \rangle|^2 = \langle \Psi | \Psi \rangle &= \langle \textstyle\sum c_{n'} f_{n'} | \sum c_n f_n \rangle \\ &= \sum_{n'} \sum_n c_{n'}^* c_n \langle f_{n'} | f_n \rangle \\ &= \sum_{n'} \sum_n c_{n'}^* c_n \delta_{nn'} \\ &= \sum_n |c_n|^2 = 1 \end{aligned}}$$

☑
$$\begin{aligned} \langle Q \rangle = \langle \Psi | \hat{Q} \Psi \rangle &= \langle \textstyle\sum_{n'} c_{n'} f_{n'} | \hat{Q} \sum c_n f_n \rangle \\ &= \langle \textstyle\sum_{n'} c_{n'} f_{n'} | \sum c_n q_n f_n \rangle \\ &= \sum c_{n'}^* c_n q_n \underbrace{\langle \psi_{n'} | \psi_n \rangle}_{\delta_{nn'}} \\ &= \sum q_n |c_n|^2 \end{aligned}$$

So... $\boxed{\langle Q \rangle = \sum_n q_n |c_n|^2}$

☑ Back to momentum, $f_p(x) = \frac{1}{\sqrt{2\pi\hbar}} \exp\left[ipx/\hbar \right]$

$$c(p,t) = \langle f_p | \Psi \rangle = \int f_p^* \Psi \, dx = \frac{1}{\sqrt{2\pi\hbar}} \int \exp\left[-ipx/\hbar\right] \Psi(x,t) dx = F^{-1}\left[\Psi(x,t)\right]_{(p)}$$

So, write

$$\boxed{\Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp\left[-ixp/\hbar\right] \Psi(x,t)\,dx = \frac{1}{\sqrt{\hbar}}\, \mathcal{F}^{-1}\left[\Psi(x,t)\right](p)}$$

↳ Momentum space Wfn

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \exp\left[ipx/\hbar\right] \phi(p,t)\,dx = \frac{1}{\sqrt{\hbar}}\, \mathcal{F}\left[\phi(p,t)\right](x)}$$

↳ position space Wfn.

$$P(dx) = |\Psi(x,t)|^2\,dx$$
$$p(dp) = |\Phi(x,t)|^2\,dx$$

Uncertainty Principle → Suppose we have observable A,

$$\sigma_A^2 = \langle \Psi | (\hat{A} - \langle A \rangle)^2 | \Psi \rangle \longrightarrow \langle A \rangle, A \text{ Hermitian} \ldots$$

$$= \langle (\hat{A} - \langle A \rangle)\Psi | (\hat{A} - \langle A \rangle)\Psi \rangle$$

Define $f = (\hat{A} - \langle A \rangle)\Psi$ For some other observable B, let $g = (\hat{B} - \langle B \rangle)\Psi$.

Then

$$\sigma_A^2 = \langle f | f \rangle, \quad \sigma_B^2 = \langle g | g \rangle .$$

So

$$\sigma_A^2 \sigma_B^2 = \langle f | f \rangle \langle g | g \rangle \geq |\langle f | g \rangle|^2$$

↳ By Schwarz Inequality

$$\|\vec{a}\|^2 \|\vec{b}\|^2 \geq |\vec{a} \cdot \vec{b}|^2$$

Pf $\quad |\gamma\rangle = |\beta\rangle - \dfrac{\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle}|\alpha\rangle$

We know $\langle\gamma|\gamma\rangle \geq 0$

So $\langle\gamma|\gamma\rangle = \left(\langle\beta| - \langle\alpha|\dfrac{\overline{\langle\alpha|\beta\rangle}}{\langle\alpha|\alpha\rangle}\right)\left(|\beta\rangle - \dfrac{\langle\alpha|\beta\rangle}{\langle\alpha|\alpha\rangle}|\alpha\rangle\right)$

$$= \langle\beta|\beta\rangle - \frac{\langle\alpha|\beta\rangle\langle\beta|\alpha\rangle}{\langle\alpha|\alpha\rangle} - \frac{\langle\alpha|\beta\rangle\langle\beta|\alpha\rangle}{\langle\alpha|\alpha\rangle} + \langle\alpha|\alpha\rangle\frac{|\langle\alpha|\beta\rangle|^2}{\langle\alpha|\alpha\rangle}$$

= [illegible] ?

Next $\langle\gamma|\beta\rangle^* = \langle\beta|\gamma\rangle = \langle\beta|\beta\rangle - \dfrac{|\langle\alpha|\beta\rangle|^2}{\langle\alpha|\alpha\rangle}$ → real

$\langle\gamma|\alpha\rangle^* = \langle\alpha|\gamma\rangle = \ldots = 0$

So $\langle\gamma|\gamma\rangle = \langle\beta|\beta\rangle - \dfrac{|\langle\alpha|\beta\rangle|^2}{\langle\alpha|\alpha\rangle} \geq 0 \Rightarrow \boxed{\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|}$

Next

$z = \langle f|g\rangle$

$|z|^2 = \mathrm{Re}^2(z) + \mathrm{Im}^2(z) \geq \mathrm{Im}^2(z) = \left(\dfrac{1}{2i}(z - z^*)\right)^2$

So $\langle f|f\rangle\langle g|g\rangle \geq |\langle f|g\rangle|^2 \geq \mathrm{Im}^2(z) = \left[\dfrac{1}{2i}\left(\langle f|g\rangle - \langle g|f\rangle\right)\right]^2$

with $\langle f|g\rangle = \langle(\hat{A} - \langle A\rangle)\Psi|(\hat{B} - \langle B\rangle)\Psi\rangle$

$$= \langle\Psi|(\hat{A} - \langle A\rangle)(\hat{B} - \langle B\rangle)\Psi\rangle$$

$$= \langle\Psi|(\hat{A}\hat{B} - \hat{A}\langle B\rangle - \langle A\rangle\hat{B} + \langle A\rangle\langle B\rangle)\Psi\rangle$$

$$= \underbrace{\langle\Psi|\hat{A}\hat{B}\Psi\rangle}_{\langle\hat{A}\hat{B}\rangle} + \underbrace{\langle\Psi|(-\hat{A}\langle B\rangle - \langle A\rangle\hat{B} + \langle A\rangle\langle B\rangle)\Psi\rangle}_{-\langle A\rangle\langle B\rangle}$$

Similarly, $\boxed{\langle g|f\rangle = \langle\hat{B}\hat{A}\rangle - \langle A\rangle\langle B\rangle}$

So $\langle f|f\rangle\langle g|g\rangle \geq \left(\dfrac{1}{2i}\left\{\langle\hat{A}\hat{B}\rangle - \langle\hat{B}\hat{A}\rangle\right\}\right)^2$

With $\langle f|g\rangle = \langle \hat{A}\hat{B}\rangle - \langle A\rangle\langle B\rangle$

$$\langle g|f\rangle = \langle \hat{B}\hat{A}\rangle - \langle A\rangle\langle B\rangle$$

So

$$\langle f|f\rangle\langle g|g\rangle \geqslant \left[\frac{1}{2i}\left(\langle\hat{A}\hat{B}\rangle - \langle\hat{B}\hat{A}\rangle\right)\right]^2$$

$$\geqslant \left[\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right]^2$$

So

$$\boxed{\sigma_A^2\sigma_B^2 \geqslant \left\{+\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right\}^2}$$

Note Commutator is anti Hermitian.

$$\boxed{\begin{aligned}\hat{Q} &= \hat{A}\hat{B} - \hat{B}\hat{A}\\ \hat{Q}^\dagger &= \hat{B}\hat{A} - \hat{A}\hat{B} = -\hat{Q}\end{aligned}} \rightsquigarrow \text{eigenvalues are } \underline{\text{imaginary}} \ldots$$

So $\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle$ is a real number $\Rightarrow \left[\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right]^2 \geqslant 0$

■ Check for $\sigma_x\sigma_p$ ...

$$\sigma_x^2\sigma_p^2 \geqslant \left[\frac{1}{2i}\langle[\hat{x},\hat{p}]\rangle\right]^2 = \left[\frac{1}{2i}(i\hbar)\right]^2 = \frac{\hbar^2}{4}$$

So $\boxed{\sigma_x\sigma_p \geqslant \frac{\hbar}{2}}$

⇒ {Can find uncertainty relation for any two operators where $[\hat{A}, \hat{B}] \neq 0$}

What does it mean for operators to (not) commute?

ct 7, 2019 ▨ If $\hat{A} \leftrightarrow \hat{B}$, then $\hat{A}(\hat{B}f) = \hat{B}(\hat{A}f) = a(\hat{B}f)$

⇒ $\hat{B}f$ is eigenfn. of $\hat{A}$, and f also eigenfn of $\hat{B}$.

⇒ $\boxed{\text{Commuting op share Eigenfunctions}}$ (compatible)

▨ If $\hat{A} \not\leftrightarrow \hat{B}$, then we call them incompatible...

Minimum Uncertainty Wave packet

- Schwarz inequality: $\langle f|f\rangle\langle g|g\rangle \geq |\langle f|g\rangle|^2$
- Also used

$$Re^2(z) + Im^2(z) \geq Im^2 z$$

- Schwarz inequality. Equality happens when $\boxed{g = cf}$
- Triangle inequality. Equality happen when $Re(z) = 0$

If $z = \langle f|g\rangle$, then want $\boxed{Re(\langle f|cf\rangle) = 0}$ ⇒

⇒ c has to be purely imaginary ⇒ $\boxed{c = ia}$

Recall... $f = (\hat{A} - \langle A\rangle)\Psi$ write $g = iaf$

$g = (\hat{B} - \langle B\rangle)\Psi$ $\hat{A} = \hat{x}$, $\hat{B} = \hat{p}$

⇒ $(\hat{p} - \langle p\rangle)\Psi = ia(\hat{x} - \langle x\rangle)\Psi$

$\boxed{(-i\hbar\partial_x - \langle p\rangle)\Psi = ia(x - \langle x\rangle)\Psi}$ → solution is a Gaussian ...

Why Gaussian? → Because Gaussian is an "eigenfn" of the Fourier transform

$$\Rightarrow \boxed{\Psi(x,t) = A\exp\left\{\frac{-a(x-\langle x\rangle)^2}{2\hbar}\right\}\cdot\exp\left\{\frac{i\langle p\rangle x}{\hbar}\right\}}$$

↳ Case with $\sigma_x\sigma_p = \frac{\hbar}{2}$ were actually Gaussian!

→ e.g. ground state of SHO...

ENERGY ~ TIME UNCERTAINTY

In special relativity, time is like space. Energy ~ momentum.

$$\hookrightarrow \boxed{\Delta E\cdot\Delta t \geqslant \frac{\hbar}{2}}$$

☒ Consider $\hat{Q} = Q(x,p,t)$. Then

$$\frac{d}{dt}\langle\hat{Q}\rangle = \frac{d}{dt}\langle\Psi|\hat{Q}|\Psi\rangle = \frac{d}{dt}\langle\Psi|\hat{Q}\Psi\rangle$$

$$= \langle\dot{\Psi}|\hat{Q}\Psi\rangle + \langle\Psi|\frac{d}{dt}(\hat{Q}\Psi)\rangle$$

$$= \langle\dot{\Psi}|\hat{Q}\Psi\rangle + \underbrace{\langle\Psi|\dot{\hat{Q}}\Psi\rangle} + \langle\Psi|\hat{Q}\dot{\Psi}\rangle$$

$$= \langle\dot{\Psi}|\hat{Q}\Psi\rangle + \langle\Psi|\hat{Q}\dot{\Psi}\rangle + \langle\dot{\hat{Q}}\rangle$$

SE $\quad i\hbar\dot{\Psi} = \hat{H}\Psi \rightarrow \dot{\Psi} = \frac{-i}{\hbar}\hat{H}\Psi$

$$\Rightarrow \frac{+i}{\hbar}\langle\hat{H}\Psi|\hat{Q}\Psi\rangle - \frac{i}{\hbar}\langle\Psi|\hat{Q}\hat{H}\Psi\rangle + \langle\dot{\hat{Q}}\rangle = \frac{d}{dt}\langle\hat{Q}\rangle$$

$$\Rightarrow \frac{i}{\hbar}\langle\Psi|\left[\hat{H},\hat{Q}\right]|\Psi\rangle + \langle\dot{\hat{Q}}\rangle = \frac{d}{dt}\langle\hat{Q}\rangle$$

So $\boxed{\frac{d}{dt}\langle \hat{Q}\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{Q}]\rangle + \langle \dot{\hat{Q}}\rangle}$

⇒ generalized Erhenfest Thm

↳ most of the time this is zero, since $\hat{Q}$ independent of time

If we have $\langle\dot{\hat{Q}}\rangle = 0$, then get

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

or $\boxed{\frac{d}{dt}\hat{Q} = \frac{i}{\hbar}[\hat{H},\hat{Q}]}$ ⇒ Heisenberg Eqn of Motion...

Erhenfest Thm   Let $\hat{Q} = \hat{p}$, we have $\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(x)$

↳ $\frac{d}{dt}\langle\hat{p}\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{p}]\rangle + \underbrace{\langle\dot{\hat{p}}\rangle}_{0}$

Look at commutator... $[\hat{H},\hat{p}] = \hat{V}p - \hat{p}\hat{V} = [\hat{V},\hat{p}]$

So $\frac{d}{dt}\langle\hat{p}\rangle = \frac{i}{\hbar}\langle[\hat{V},\hat{p}]\rangle$

Next, look at $[\hat{V},\hat{p}]f = \hat{V}\hat{p}f - \hat{p}\hat{V}f$

$$= \hat{V}(-i\hbar\partial_x)f + i\hbar\partial_x(Vf)$$

$$= V(\cancel{-i\hbar\partial_x f}) + i\hbar(\partial_x V)f + \cancel{i\hbar V(\partial_x f)}$$

$$= i\hbar(\partial_x V)f$$

So $[\hat{V},\hat{p}] = i\hbar\partial_x V$

So $\boxed{\frac{d}{dt}\langle\hat{p}\rangle = \frac{i}{\hbar}\langle(i\hbar)\partial_x V\rangle = \langle-\partial_x V\rangle}$ ⇝ Erhenfest Thm

Back to energy & time

$$\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i}\langle[\hat{A},\hat{B}]\rangle\right)^2$$

If $\hat{A}=\hat{H}$, and $\hat{B}=\hat{Q}$, then

$$\sigma_H^2 \sigma_Q^2 \geq \left(\underbrace{\frac{1}{2i}\langle[\hat{H},\hat{Q}]\rangle}\right)^2$$

$$\sigma_H^2 \sigma_Q^2 \geq \left(\frac{\hbar}{2}\right)^2\left(\frac{d}{dt}\langle\hat{Q}\rangle\right)^2$$ assuming $\langle\dot{\hat{Q}}\rangle = 0$

↳ $$\boxed{\sigma_H \sigma_Q \geq \frac{\hbar}{2}\frac{d}{dt}\langle\hat{Q}\rangle}$$

Since $\langle\hat{H}\rangle = E$, $\sigma_H = \sigma_E = \Delta E$

Let $\sigma_Q = \left|\frac{d}{dt}\langle\hat{Q}\rangle\right|\Delta t = \Delta Q$

So $$\boxed{\Delta E \Delta t \geq \frac{\hbar}{2}}$$

Δt is the time for an expectation value to change by 1σ

Oct 9, 2019

BASES

Some state vector $|S(t)\rangle$, then

$$\boxed{\begin{array}{c} \Psi(x,t) = \langle x | S(t)\rangle \\ \hline \Phi(p,t) = \langle p | S(t)\rangle \\ \hline c_n(t) = \langle n | S(t)\rangle \end{array}}$$

&

$$|S(t)\rangle = \int \Psi(y,t)\,\delta(y-x)\,dx$$
$$= \int \Phi(p,t)\frac{1}{\sqrt{2\pi\hbar}}\exp\left\{\frac{ipx}{\hbar}\right\}dp$$
$$= \sum c_n \exp\left\{-iE_n t/\hbar\right\}\psi_n(x)$$

↳ analogously... If $|\alpha\rangle = \sum a_n|e_n\rangle$, $|\beta\rangle = \sum b_n |e_n\rangle$ (ONB)

↳ $a_n = \langle e_n|\alpha\rangle$; $b_n = \langle e_n|\beta\rangle$. Operator → matrix

$\hat{Q}$ ~ operator ⇒ matrix

$$\boxed{Q_{mn} \equiv \langle e_m|\hat{Q}|e_n\rangle}$$

Let $|\beta\rangle = \hat{Q}|\alpha\rangle$ but $|\beta\rangle = \sum b_n|e_n\rangle = \sum a_n \hat{Q}|e_n\rangle$

Then $\sum b_n \underbrace{\langle e_m|e_n\rangle}_{\delta_{mn}} = \sum a_n \langle e_m|\hat{Q}|e_n\rangle$

So $\boxed{b_m = \sum_n Q_{mn} a_n}$

$\boxed{\text{Ex}}$ Two-state system

Two independent states $|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $|2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

General state: $S = a|1\rangle + b|2\rangle$, $|a|^2 + |b|^2 = 1$.

Write Hamiltonian as matrix:

$$\hat{H} = \begin{pmatrix} h & g \\ g & h \end{pmatrix}$$ where h, g real constants..

- At $t=0$, $|S\rangle = |1\rangle$.
- SE $i\hbar\partial_t|S\rangle = \hat{H}|S\rangle$. Need to find eigenstates of $\hat{H}$.

$$\hat{H}|\sigma\rangle = E|\sigma\rangle$$

↳ $E_\pm = h \pm g$; $|\sigma_\pm\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$

So $|S(0)\rangle = \frac{1}{\sqrt{2}}\{|\sigma_+\rangle + |\sigma_-\rangle\}$ ⇒ ~~$|S(t)\rangle = \frac{1}{\sqrt{2}}\{|\sigma_+\rangle + |\sigma_-\rangle\}$~~

So $$|S(t)\rangle = \frac{1}{2} e^{-i(h+g)t/\hbar}\begin{pmatrix}1\\1\end{pmatrix} + \frac{1}{2}\exp^{-i(h-g)t/\hbar}\begin{pmatrix}1\\-1\end{pmatrix}$$

$$\boxed{|S(t)\rangle = e^{iht/\hbar}\left\{\begin{matrix}\cos(gt/\hbar)\\ -i\sin(gt/\hbar)\end{matrix}\right\}}$$

//

More Brakets... $|\alpha\rangle = \begin{pmatrix}a_1\\ \vdots\\ a_N\end{pmatrix}$; $\langle\beta| = (b_1^* \dots b_N^*)$ ⇝ dual of kets...

$$\boxed{\langle\beta|\alpha\rangle = \sum a_n b_n^*}$$

Projection operator $\boxed{\hat{P}_\alpha = |\alpha\rangle\langle\alpha|}$

projects $|\beta\rangle$ along $|\alpha\rangle$

$$\hat{P}_\alpha|\beta\rangle = |\alpha\rangle\langle\alpha|\beta\rangle = \langle\alpha|\beta\rangle|\alpha\rangle$$

For a complete ONB $\{e_N\}$

$$\boxed{\sum_n |e_n\rangle\langle e_n| = 1} \longrightarrow \text{completeness} \quad \langle e_n|e_m\rangle = \delta_{mn}$$

or

$$\boxed{\int |e_n\rangle\langle e_n| dn = 1} \longrightarrow \text{completeness} \quad \langle e_n|e_m\rangle = \delta(n-m)$$

$$|\alpha\rangle = \sum_n \langle e_n|\alpha\rangle|e_n\rangle$$

Really should be... $\langle f|\hat{Q}f\rangle \rightsquigarrow \langle f|\hat{Q}|f\rangle$

↳ looks like $\langle f|(\hat{Q}|f\rangle)$ or $(\langle f|\hat{Q}^\dagger)|f\rangle$

Some properties $(\hat{Q}+\hat{R})|\alpha\rangle = \hat{Q}|\alpha\rangle + \hat{R}|\alpha\rangle$

$$\hat{Q}\hat{R}|\alpha\rangle = \hat{Q}\left(\hat{R}|\alpha\rangle\right)$$

Functions of operator $\exp[\hat{Q}] = \sum_{n=0}^{\infty} \frac{\hat{Q}^n}{n!}$

$$\frac{1}{1-\hat{Q}} = \sum_{n=0}^{\infty} \hat{Q}^n$$

$$\ln \hat{Q} = \sum_{n=1}^{\infty} -\frac{\hat{Q}^n}{n} \cdot (-1)^n$$

Transforms ..

$$\left\{ \begin{aligned} 1 &= \int |x\rangle\langle x|\,dx \\ 1 &= \int |p\rangle\langle p|\,dp \\ 1 &= \sum |n\rangle\langle n| \end{aligned} \right\}$$

$$\Rightarrow \quad |S(t)\rangle = \int |x\rangle\langle x|\,dx\,|S(t)\rangle = \int \underbrace{\langle x|S(t)\rangle}_{\Psi(x,t)} |x\rangle\,dx$$

$$\boxed{|S(t)\rangle = \int \Psi(x,t)\,|x\rangle\,dx}$$

Start with $\Phi(p,t) = \langle p|S(t)\rangle$

$$= \langle p| \int |x\rangle\langle x|\,dx\,|S(t)\rangle$$

$$= \int \langle p|x\rangle \underbrace{\langle x|S(t)\rangle}\,dx$$

$$= \int \langle p|x\rangle\,\Psi(x,t)\,dx$$

$\langle x|p\rangle \sim$ momentum eigenstate in position space...

$$\boxed{\langle x|p\rangle = f_p = \frac{1}{\sqrt{2\pi\hbar}} \exp\left[\frac{ipx}{\hbar}\right]}$$

So

$$\Phi(p,t) = \int \Psi(x,t)\, \frac{1}{\sqrt{2\pi\hbar}}\, e^{-ipx/\hbar}\, dx = F^{-1}\left[\Psi(x,t)\right]$$

Make sure operators are in the right basis...

$$\boxed{\begin{aligned} \hat{x} &= \begin{cases} (x) & \text{in position space ...} \\ (i\hbar\partial_p) & \text{in momentum space} \end{cases} \\ \hat{p} &= \begin{cases} (-i\hbar\partial_p) & \text{in position space} \\ (p) & \text{in momentum space} \end{cases} \end{aligned}}$$

So

$$\langle x|\hat{x}|S(t)\rangle = x\,\Psi(x,t)$$

...

$$\langle p|\hat{x}|S(t)\rangle = i\hbar\partial_p\,\Phi(p,t)$$

Ex Look at $\langle p|\hat{x}|S(t)\rangle$ ...

$$\begin{aligned} \langle p|\hat{x}|S(t)\rangle &= \langle p|\hat{x}\int |x\rangle\langle x|\,dx\,|S(t)\rangle \\ &= \int \underline{\langle p|\hat{x}|x\rangle}\ \underline{\langle x|S(t)\rangle}\,dx \qquad \hat{x}|x\rangle = x|x\rangle \\ &= \int x\,\underline{\langle p|x\rangle}\,\langle x|S(t)\rangle\,dx \\ &= \int x\,\Psi(x,t)\,e^{-ipx/\hbar}\,dx \\ &= \frac{1}{\sqrt{2\pi\hbar}}\int (+i\hbar\partial_p)\,e^{-ipx/\hbar}\cdot\Psi(x,t)\,dx \\ &= F^{-1}\left[i\hbar\partial_p\,\Psi(x,t)\right]dx = \boxed{i\hbar\partial_p\,\Phi(p,t)} \end{aligned}$$

$\hat{x} \sim i\hbar\partial_p$ in momentum space

✓

SCHRÖDINGER EQUATION IN 3D

Oct 10, 2019

Time dependent : $\hat{H}\Psi : i\hbar\partial_t\Psi$

☒ $$\boxed{\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})}$$

Cartesian : $\nabla^2 = \partial_x^2 + \partial_y^2 + \partial_z^2$

Spherical : $\nabla^2 = \frac{1}{r^2}\partial_r(r^2\partial_r) + \frac{1}{r^2\sin\theta}\partial_\theta(\sin\theta\,\partial_\theta) + \frac{1}{r^2\sin^2\theta}\partial_\varphi^2$

θ : polar $0-\pi$

φ : Azimuthal $0-2\pi$

☒ Momentum : $\boxed{\vec{p} = -i\hbar\vec{\nabla}}$

☒ Normalization : $1 = \int|\Psi|^2 d^3r = \int|\Psi|^2 r^2\sin\theta\,d\theta\,dr\,d\varphi$

$= \int|\psi|^2 r^2 d(\cos\theta)\,d\varphi$

☒ Time dependence → same! $\Psi(r,t) = \psi_n(x)\exp\left[-iE_nt/\hbar\right]$

☒ SE :

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{r})\psi = E\psi$$

$$\Psi(r,t) = \sum_{n=0}^{\infty} c_n\psi_n\exp\{-iE_nt/\hbar\}$$

☒ Most potentials are central potentials $V(\vec{r}) = V(r)$

<u>In spherical coords</u>

$$-\frac{\hbar^2}{2m}\left\{\frac{1}{r^2}\partial_r(r^2\partial_r) + \frac{1}{r^2\sin\theta}\partial_\theta(\sin\theta\,\partial_\theta) + \frac{1}{r^2\sin^2\theta}\partial_\varphi^2\right\}\psi + V\psi = E\psi \qquad \psi = \psi(r,\theta,\varphi)$$

$V = V(r)$

Assume $\boxed{\Psi(r,\theta,\varphi) = R(r)Y(\theta,\varphi)}$

Apply to $R(r)\,Y(\theta,\varphi)$, and divide, to get ... multiplied r^2

$$-\frac{\hbar^2}{2m}\frac{1}{R}\left\{\frac{1}{r^2}\partial_r(r^2\partial_r)\right\}R + \frac{-\hbar^2}{2m}\frac{1}{Y}\left\{\frac{1}{r^2\sin\theta}\partial_\theta(\sin\theta\,\partial_\theta) + \frac{1}{r^2\sin^2\theta}\partial_\varphi^2\right\}Y + V(r) = E$$

So, $$-\frac{\hbar^2}{2m}\frac{1}{R}\left\{\frac{1}{r^2}\partial_r(r^2\partial_r)\right\}R + V(r) - E = \frac{1}{Y}\frac{\hbar^2}{2m}\left\{\frac{1}{r^2\sin\theta}\partial_\theta(\sin\theta\,\partial_\theta) + \frac{1}{r^2\sin^2\theta}\partial_\varphi^2\right\}Y$$

$$\hookrightarrow \frac{1}{R}\left\{\partial_r(r^2\partial_r)\right\}R - \frac{2mr^2}{\hbar^2}\left(V(r)-E\right) = \frac{-1}{Y}\left[\frac{1}{\sin\theta}\partial_\theta(\sin\theta\,\partial_\theta)Y + \frac{1}{r^2\sin^2\theta}\partial_\varphi^2 Y\right]$$

Call seperation constant $\boxed{\ell(\ell+1)}$

Radial Eqn $$\boxed{\partial_r(r^2\partial_r)R - \frac{2mr^2}{\hbar^2}\left(V(r)-E\right) = \ell(\ell+1)R}$$

Angular Eqn $$\boxed{\sin\theta\,\partial_\theta(\sin\theta\,\partial_\theta Y) + \partial_\varphi^2 Y = -\ell(\ell+1)Y\sin^2\theta}$$

Focus on Angular Solution $Y(\theta,\varphi) = \Theta(\theta)\,\Phi(\varphi)$

Then ... $$\left[\frac{1}{\Theta}\left\{\sin\theta\,\partial_\theta(\sin\theta\,\partial_\theta\,\Theta\right\} + \frac{\partial_\varphi^2\Phi}{\Phi} = -\ell(\ell+1)\sin^2\theta\right]$$

Seperation constant: $\boxed{m^2}$

So $$\boxed{\sin\theta\,\partial_\theta(\sin\theta\,\partial_\theta)\Theta + \ell(\ell+1)\sin^2\theta\,\Theta = m^2\Theta}$$

$$\boxed{\partial_\varphi^2\Phi = -m^2\Phi}$$

Solution to Φ equation is $\boxed{\Phi(\varphi) = \exp\{im\phi\}} \xrightarrow{} m\in\mathbb{Z}$

Wait $\Phi(\varphi) = \Phi(\varphi+2\pi) \Rightarrow \boxed{m\in\mathbb{Z} = 0, \pm1, \pm2, \dots\ (?)}$

Ⓗ equation $\sin\theta\, \partial_\theta (\sin\theta\, \partial_\theta)\, Ⓗ + l(l+1) \sin^2\theta\, Ⓗ = m^2\, Ⓗ$

$$\Rightarrow \boxed{\sin\theta\, \partial_\theta (\sin\theta\, \partial_\theta) + (l(l+1) \sin^2\theta - m^2)\, Ⓗ = 0}$$

$$Ⓗ(\theta) = A P_l^m (\cos\theta)$$ → associated Legendre polynomials

Legendre polynomials? Let $x = \cos\theta$, then $x \in [-1, 1]$

$$\boxed{\frac{d}{dx}\left[(1-x^2)\frac{dP}{dx}\right] - l(l+1) P = 0}$$

Assume power series solution...

$$P(x) = x^\alpha \sum_{j=0}^{\infty} a_j x^j$$

So...
$$\sum_{j=0}^{\infty}\left[(\alpha+j)(\alpha+j-1)\, a_j x^{\alpha+j-2} - \left\{(\alpha+j)(\alpha+j-1) - l(l+1)\right\} a_j x^{\alpha+j}\right] = 0$$

Index shifting... then require vanishing

Recursion relation... $$\boxed{a_{j+2} = \frac{(\alpha+j)(\alpha+j-1) - l(l+1)}{(\alpha+j+1)(\alpha+j+2)}\, a_j}$$

⊕ If $a_0 \neq 0$, then $\alpha(\alpha-1) = 0$ ($j=1$ terms must be 0)
($j=0$)

⊕ If $a_1 \neq 0$, then $\alpha(\alpha+1) = 0$ ($j=0$ terms must be 0)
($j=1$)

(†) If we pick $j=0$ terms $\neq 0$, then $\alpha(\alpha-1) = 0 \Rightarrow \alpha = 0$ or $\alpha = 1$

If $\alpha = 0$, then $P(x) = \sum_{j=0}^{\infty} a_j x^j$. If $\alpha = 1$, then $\sum_{j=0}^{\infty} a_j x^{j+1}$

(†) If $j=1$ term $\neq 0$, then $\alpha(\alpha+1) = 0 \Rightarrow \alpha=0$ or $\alpha=-1$

$$\alpha = 0 \longrightarrow P(x) = \sum_{j=0}^{\infty} a_j x^j$$

$$\alpha=-1 \longrightarrow P(x) = \sum_{j=0}^{\infty} a_j x^{j-1} \rightarrow P(x) = \sum_{j=1}^{\infty} a_j x^j$$

(★) Recognize that $P(x)$ @ $\alpha=0$ same
$P(x)$ @ $\alpha=\pm1$ same

$\Rightarrow$ pick $\alpha=0 \Rightarrow$ get simpler recursion...

$$\boxed{a_{j+2} = \frac{j(j+1)-\ell(\ell+1)}{(j+1)(j+2)}\, a_j}$$

st 11, 2019

f. $P(x) = \sum a_j x^j$ with even ; odd ... but picking one is fine.

Need this to converge from $[-1, 1]$.

$$\frac{a_{j+2}\, x^{j+2}}{a_j x^j} = \frac{j(j+1)-\ell(\ell+1)}{(j+1)(j+2)}\, x^2 \xrightarrow{j\to\infty} x^2 \rightarrow 0$$

for $x \in (-1,1$

But doesn't converge at $-1, 1 \Rightarrow$ need to truncate series...

Which requires $\boxed{j(j+1) = \ell(\ell+1)} \rightarrow \ell$ must be 0 or positive int

$\ell = 0, 1, 2, 3, \ldots$

Convention: $P_\ell(1) = 1$.

Prove orthogonality

$$\frac{d}{dx}\left\{(1-x^2)\frac{dP_\ell}{dx}\right\} + (\ell+1)\ell P_\ell = 0 \rightsquigarrow$$

$$\int_{-1}^{1} dx \left[P_{l'} \frac{d}{dx}\left((1-x^2)\frac{d}{dx}P_l\right)\right] + P_{l'}\, l(l+1) P_l = 0$$

= Integration by parts...

$$= \int_{-1}^{1} dx \left\{ (x^2-1) \frac{dP_l}{dx}\frac{dP_{l'}}{dx} + l(l+1) P_{l'} P_l \right\} = 0$$

Do this again with $l \mapsto l'$

So $$\int_{-1}^{1} dx \left\{ (x^2-1) \frac{dP_{l'}}{dx}\frac{dP_l}{dx} + l'(l'+1) P_l P_{l'} \right\} = 0$$

Add / Subtract $\Rightarrow$ $$\int_{-1}^{1} dx \left[l'(l'+1) - l(l+1) \right] P_l P_{l'} = 0$$

So either $l = l'$ or $\int_{-1}^{1} P_l P_{l'} = 0 \Rightarrow P_l \perp P_{l'}$

When $l = l'$,

$$\boxed{\int_{-1}^{1} P_{l'} P_l \, dx = \frac{2}{2l+1} \delta_{l'l}}$$

Associated Legendre Polynomials

$$\boxed{\frac{d}{dx}\left[(1-x^2) \frac{d}{dx} P \right] + \left\{ l(l+1) - \frac{m^2}{1-x^2} \right\} = 0}$$

Now we have P_l^m, Do same thing... multiply by $P_{l'}^{m'}$ and integrate, then swap $m \leftrightarrow m'$, $l \leftrightarrow l'$ and subtract...

$$\hookrightarrow \boxed{\left[l(l+1) - l'(l'+1) \right] \int_{-1}^{1} P_l^m P_{l'}^{m'} \, dx - (m^2 - m'^2) \int_{-1}^{1} \frac{1}{1-x^2} P_{l'}^{m'} P_l^m \, dx = 0}$$

For $m = m'$, get

$$\boxed{\int_{-1}^{1} dx \; P_{\ell'}^{m} P_{\ell}^{m} = \frac{2(\ell+m)!}{(2\ell+1)(\ell-m)!}\,\delta_{\ell\ell'}}$$

For fixed ℓ $(\ell=\ell')$

$$\boxed{\int_{-1}^{1} dx \; \frac{1}{1-x^2} P_{\ell}^{m} P_{\ell}^{m'} dx = \begin{cases} 0 & \text{if } \quad m \neq m' \\ \dfrac{(\ell+m)!}{m(\ell-m)!} & m = m' \neq 0 \\ \infty & m = m' = 0 \end{cases}}$$

Associated legendre polynomials are the solution to the Θ piece of the angular wavefunction...

So $$\boxed{Y_{\ell}^{m}(\theta,\phi) = \sqrt{\frac{(2\ell+1)(\ell-m)!}{\cancel{4\pi}(\ell+m)!}}\; \exp\left[+im\phi\right] P_{\ell}^{m}(\cos\theta)}$$ → spherical harmonics

$\ell = 0, 1, 2, 3, \ldots$
$m = -\ell \ldots 0 \ldots \ell$

normalization...

Normalization...

$$\int_0^{2\pi}\int_0^{\pi} \sin\theta \, d\theta \, d\phi \; Y_{\ell}^{m*}(\theta,\varphi)\, Y_{\ell}^{m}(\cancel{\theta}\varphi) = 1$$

$\underline{\psi}$

RADIAL PART ⇒ normalise independently $\int_{\cancel{0}}^{\infty} R^{*}(r) R(r)\, r^2 dr = 1$

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

Define $u(r) = rR(r)$

$$\Rightarrow \frac{dR}{dr} = \frac{1}{r^2}\left[r\frac{du}{dr} - u\right] \Rightarrow \frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) = r\frac{d^2u}{dr^2}$$

So, eqn becomes...

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

↳ This is basically an SE with $V_{eff} = V(r) + \underbrace{\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}}_{\text{centrifugal term}}$

then we get

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + V_{eff}\,u = Eu}$$

Normalization cond. for u: $\int_{0}^{\infty}|R|^2 r^2 dr = \int_0^{\infty}|u|^2 dr = 1$

<u>What is V_{eff}?</u>

↳ Start with ...

INFINITE SPHERICAL WELL

$$V(r) = \begin{cases} 0 & r \le a \\ \infty & r > a \end{cases}$$

Solve this problem gives...

$$\frac{d^2u}{dr} = \left[\frac{l(l+1)}{r^2} - k^2\right]u \qquad k = \frac{\sqrt{2mE}}{\hbar}$$

If $l = 0$, get sines & cosines like before...

If $l \neq 0$, $\boxed{u(r) = \left(A j_l(kr) + B n_l(kr)\right)r} \longrightarrow$ ✪

$j_l \rightarrow$ spherical Bessel function

$n_l \rightarrow$ spherical Neumann function

Bessel functions...

$$\boxed{\begin{aligned} j_\ell(x) &= (-x)^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\sin(x)}{x} \\ n_\ell(x) &= -(-x)^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\cos(x)}{x} \end{aligned}}$$

Ex $\quad j_0 \sim \frac{\sin x}{x} \qquad n_0 = -\frac{\cos x}{x}$

$j_1 \sim \frac{\sin x}{x^2} - \frac{\cos x}{x} \quad \ldots$

Note Neumann functions blow up at $r=0 \Rightarrow B=0$

So $\quad u(r) = A j_r(kr) \cdot r \Rightarrow \boxed{R(r) = A j_\ell(kr)}$

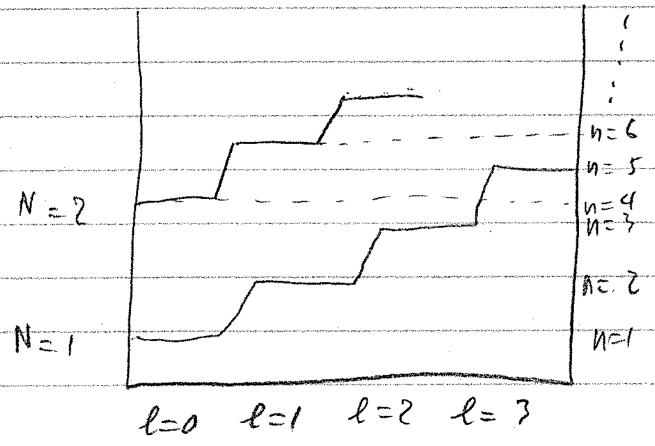
Want $\quad R(a) = 0$

↳ let $k = \frac{1}{a}\beta_{N,\ell} \rightsquigarrow N^{th}$ zero at the ℓ^{th} Bessel

Then $\boxed{E_{N\ell} = \frac{\hbar^2}{2ma^2}\beta_{N,\ell}^2}$

So full wfn is...

$$\boxed{\psi_{n\ell m}(r,\theta,\varphi) = A_{n\ell}\, j_\ell\left(\beta_{N\ell}\, r/a\right) Y_\ell^m(\theta,\varphi)} \rightsquigarrow \text{for } V_{eff} = \delta$$



$n = 1,2,3$ are the $N=1$ zeros of $\ell = 0,1,2\ldots$

$n=4$ is the $N=2$ zero of $\ell=0$.

HYDROGEN

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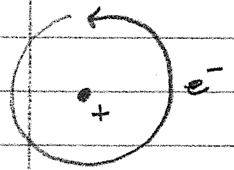
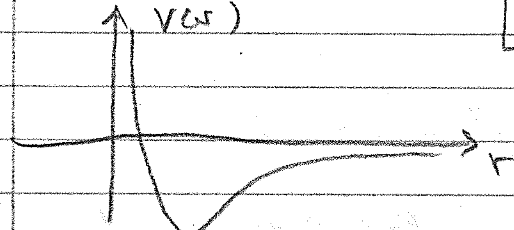


$$V(r) = \frac{-e^2}{4\pi\varepsilon_0}\frac{1}{r}$$

SE (radial)

$$\boxed{\frac{-\hbar^2}{2m_e}\frac{d^2u}{dr} + \left[\frac{-e^2}{4\pi\varepsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m_e}\frac{(l)(l+1)}{r^2}\right]u = Eu}$$



there both bound & scattering states

E<0 E>0

↳ Interested in bound states.

Angular piece → spherical harmonics...

write $k = \frac{\sqrt{-2mE}}{\hbar}$

Got $$\frac{1}{k^2}\frac{d^2u}{dr^2} = \left\{1 - \frac{m_e e^2}{2\pi\varepsilon_0\hbar^2 k}\frac{1}{r} + \frac{(l)(l+1)}{(kr)^2}\right\}u$$

Define $\rho = kr$, $\rho_0 = \frac{m_e e^2}{2\pi\varepsilon_0\hbar^2 k}$

↳ get $$\frac{d^2u}{d\rho^2} = \left\{1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right\}u$$

When $\rho \to \infty$, $u \simeq A\exp\{-\rho\} + \overset{0}{\cancel{B\exp\{\rho\}}} = A\exp\{-\rho\}$

So $\boxed{u(\rho) = Ae^{-\rho}}$ @ $\rho \to \infty$

when $\rho \to 0$, $\frac{l(l+1)}{\rho^2}$ dominates... (centrifugal term...)

$$\frac{d^2u}{d\rho^2} = \frac{l(l+1)}{\rho^2}u \Rightarrow \boxed{u(\rho) = C\rho^{l+1} + \underset{0}{\cancel{D\rho^{-l}}}}$$

So $\boxed{u(\rho) = C\rho^{l+1}}$ → when ρ small...

Write u(ρ) as asymptotic behavior times polynomial ...

So $\boxed{u(\rho) = \rho^{l+1} \exp\{-\rho\}\, V(\rho)} \rightarrow$ polynomials...

So $$\frac{du}{d\rho} = \rho^{l} \exp\{-\rho\} \left\{ (l+1-\rho)V + \rho \frac{dV}{d\rho} \right\}$$

And $$\frac{d^2u}{d\rho^2} = \rho^{l} \exp\{-\rho\} \left\{ \left(-2l-2+\rho+\frac{(l+1)l}{\rho}\right)V + 2(l+1-\rho)\frac{dV}{d\rho} + \rho\frac{d^2V}{d\rho^2} \right\}$$

So... new radial eqn... in terms of V(ρ)

$$\boxed{\rho\frac{d^2V}{d\rho^2} + 2(l+1-\rho)\frac{dV}{d\rho} + (\rho_0 - 2(l+1))V = 0}$$

Use power series solution... $V(\rho) = \sum c_j \rho^j$

So $$\frac{dV}{d\rho} = \sum j c_j \rho^{j-1} = \sum (j+1) c_{j+1} \rho^j$$

$$\frac{d^2V}{d\rho^2} = \sum j(j+1) c_{j+1} \rho^{j-1}$$

Putting all these together & simplify...

$$\sum j(j+1)c_{j+1}\rho^j + \sum (2)(l+1)(j+1)c_{j+1}\rho^j - 2\sum j c_j \rho^j + (\rho_0 - 2(l+1))\sum c_j \rho^j = 0$$

⇒ get recursion relation between c_j & c_{j+1} ...

$$j(j+1)c_{j+1} + 2(l+1)(j+1)c_{j+1} - 2jc_j + (\rho_0 - 2(l+1))c_j = 0$$

Solve for $c_{j+1} \sim c_j$

$$\boxed{c_{j+1} = \left\{ \frac{2(j+\ell+1) - \rho_0}{(j+1)(j+2\ell+2)} \right\} c_j} \qquad \ell = 0, 1, 2, 3, \ldots$$

Need series to terminate @ N such that $N-1 \neq 0$ but $N = 0$

Highest $j = N-1$.

$$\hookrightarrow \quad 2\{\overset{+\ell}{N-1+1}\} - \rho_0 = 0 \Rightarrow 2(N+\ell) = \rho_0 \rightarrow \boxed{n = \rho_0/2} \quad n = N+\ell$$

where $\rho_0 = \dfrac{m_e e^2}{2\pi\varepsilon_0 \hbar^2 k} = \dfrac{m_e e^2}{2\pi\varepsilon_0 \hbar \sqrt{-2m_e E}} = 2(N+\ell)$

$$\rightarrow E = \frac{-M_e e^4}{8\pi^2 \varepsilon^2 \hbar^2 \rho_0^2}$$

or

$$\boxed{E = -\left\{ \frac{m_e}{2\hbar^2} \left(\frac{e^2}{4\pi\varepsilon_0} \right)^2 \frac{1}{n^2} \right\} = \frac{E_1}{n^2}}$$

From Bohr model

$E_1 = -13.6\,\text{eV}$, $n = 1, 2, 3, \ldots$

Define Bohr radius... $\boxed{K = \left(\dfrac{m_e e^2}{4\pi\varepsilon_0 \hbar^2} \right) \dfrac{1}{n} = \dfrac{1}{a_0 n}}$

$$\boxed{a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{m_e e^2} \sim 0.529\,\text{Å}}$$

Because $\rho = kr$, $\boxed{\rho = \dfrac{r}{a_0 n}}$

So, radial wfn...

$$\frac{u}{r} \leftarrow \boxed{R_{n\ell}(r) = \frac{1}{r} \overbrace{\rho^{\ell+1} \exp\{-\rho\} V(\rho)}^{u(\rho)}}$$

So...

Full wfn...

$$\psi_{n\ell m_\ell}(r,\theta,\varphi) = \frac{1}{r}\rho^{\ell+1}e^{-\rho}v(\rho)\,Y_\ell^{m_\ell}(\theta,\varphi)$$

where $v(\rho)$ is an $n-\ell-1$ degree polynomial in $\rho = \frac{r}{a_0 n}$

If we put n into recursion relation for c_j...

$$\frac{2(j+\ell+1-n)}{(j+1)(j+2\ell+2)}c_j = c_{j+1} \qquad j = 0,1,2,\ldots$$

Max allowed $j = n-\ell-1$.

For $n=1$, can only have $\ell=0$

$$\Rightarrow n>\ell, \quad -\ell \le m \le \ell$$

Ground state

$$n=1, \quad \ell=0, \quad m=0.$$

$$\psi_{100}(r,\theta,\varphi) = R_{10}(r)\,Y_0^0(\theta,\varphi)$$

$$= R_{10}(r)\left(\frac{1}{4\pi}\right)^{1/2}$$

$$= \frac{1}{r}\left(\rho\exp(-\rho)\,c_0\right)\left(\frac{1}{4\pi}\right)^{1/2} \qquad \rho = \frac{r}{a_0 n}$$

$$= \frac{1}{a_0}c_0\,\cancel{\rho}\exp(-\rho)\left(\frac{1}{4\pi}\right)^{1/2}$$

Then find c_0 by ~~[illegible]~~ Normalizing...

$$c_0 = \frac{2}{\sqrt{a_0}} \Rightarrow \psi_{100}(r,\theta,\varphi) = \frac{2}{\sqrt{a_0}}\exp\left\{\frac{-r}{a_0^{3/2}}\right\}\left(\frac{1}{4\pi}\right)^{1/2}$$

$$\boxed{\psi_{100}(r,\theta,\varphi) = \frac{1}{\sqrt{\pi a^3}}\exp\left(-r/a_0\right)}$$

Power series we found → called associated Laguerre polynomials

$$\boxed{L_q^{\,p}(x) = (-1)^p \left(\frac{d}{dx}\right)^p L_{p+q}(x)}$$

where the regular polynomial ...

$$\boxed{L_q(x) = \frac{e^x}{q!}\left(\frac{d}{dx}\right)^q \left[e^{-x}\cdot x^q\right]}$$

As usual, these polyns are orthogonal, complete, ...

In general, ... can write ψ_{nlm_l} wfn. as

$$\boxed{\begin{aligned}\psi_{nlm_l}(r,\theta,\phi) &= \sqrt{\frac{(n-l-1)!}{(2n)(n+l)!}\left(\frac{2}{na_0}\right)^3}\ \exp\left\{\frac{-r}{na_0}\right\} \\ &\quad \times \left(\frac{2r}{na_0}\right)^l \left[L^{2l+1}_{n-l-1}\left(\frac{2r}{na}\right)\right] Y_l^m(\theta,\phi)\end{aligned}}$$

<u>Orthogonality</u>

$$\int \psi^*_{nlm_l}\,\psi_{n'l'm_{l'}}\,d^3r = \delta_{nn'}\,\delta_{mm'}\,\delta_{ll'}$$

Each state is described by 3 quantum numbers...

$$\left\{\begin{array}{l} n:\ \text{Principal quantum number.} \\ l:\ \text{Azimuthal quantum number.} \\ m_l:\ \text{magnetic quantum number} \end{array}\right\}\ \text{angular momentum}$$

$$\boxed{\begin{array}{ll} n = 1, 2, 3 \ldots & \\ l = 0, \ldots n-1 & 0 \le l < n, \quad -l \le m \le l \\ m = -l \ldots 0 \ldots l & \end{array}}$$

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Recall wfn

$$\boxed{\begin{array}{l} \psi_{nlm_\ell}(r,\theta,\varphi) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n(n+\ell)!}} \exp\left[\frac{-r}{na_0}\right] \cdot \left(\frac{2r}{na_0}\right)^\ell \left\{ L^{2n+\ell}_{n-\ell-1}\left(\frac{2r}{na_0}\right) Y_\ell^m(\theta,\varphi \right. \\ \\ \text{where} \quad n = 1, 2, 3, \ldots \quad \ell = 0, 1, \ldots n-1 \quad , E_n = \frac{E_1}{n^2} \\ \qquad\qquad\qquad -\ell \leq m \leq \ell \end{array}}$$

Energy depends only on n. For $n > 1$, get degeneracy ...

Ex $n = 2 \Rightarrow \ell = 0,\ m = 0$

$\ell = 1,\ m = -1, 0, 1$

▨ In general, (without spin) for each n, n^2 degeneracies...

$$\text{Total degeneracy} = \boxed{\sum_{\ell=0}^{n-1} (2\ell+1) = n^2} \longrightarrow \text{without spin} \ldots$$

Possible bound state energies is given by $E_n = \frac{E_1}{n^2}$.

→ There're an infinite number of bound states.

→ spacing gets smaller as n increases.

Define $E_\infty = 0$ → separate bound from scattering states...

▨ Note Laguerre polynomials always have c_0 in them...
Find c_0 by normalization.

ANGULAR MOMENTUM

Recall $\vec{L} = \vec{r} \times \vec{p} \rightarrow \left\{ \begin{array}{l} L_x = yp_z - zp_y \\ L_y = zp_x - xp_z \\ L_z = xp_y - yp_x \end{array} \right\}$

In quantum, there are operators... Note Operators that commute share eigen-spaces...

Check if these commute...

$$[L_x, L_y] = [yp_z - zp_y, \; zp_x - xp_z]$$

$$= [yp_z, zp_x] + \cancelto{0}{[-zp_y, zp_x]} - \cancelto{0}{[yp_z, xp_z]} + [zp_y, xp_z]$$

x, y, z and p_x, p_y, p_z all commute...

....

Expand to get $[L_x, L_y] = y\underbrace{[p_z, x]}p_x + x\underbrace{[z, p_z]}p_y$

$$= -i\hbar(\underbrace{yp_x - zp_y}_{-L_z}) = +i\hbar L_z$$

So $\boxed{[L_x, L_y] = -i\hbar L_z}$

Generally $\boxed{[L_\alpha, L_\beta] = i\hbar \, \varepsilon_{\alpha\beta\gamma} L_\gamma} \rightsquigarrow$ none commute.

Levi-Civita symbol?

$$\varepsilon_{\alpha\beta\gamma} = \begin{cases} 1 & \alpha\beta\gamma = 123, \; 231, \; 312 \quad \text{(cyclic)} \\ 0 & \text{if any 2 indices same} \\ -1 & \alpha\beta\gamma = 132, \; 321, \; 213 \quad \text{(cyclic)} \end{cases}$$

But L^2 commutes with all of them...

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

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

$$= 0 + L_y[L_y, L_x] + [L_y, L_x]L_y$$

$$+ L_z[L_z, L_x] + [L_z, L_x]L_z$$

$$= L_y(-i\hbar L_z) + (-i\hbar L_z)L_y + (i\hbar L_y)L_z + L_z(i\hbar L_y)$$

$$\boxed{[L^2, L_x] = 0}$$

In general $\boxed{[L^2, \vec{L}] = 0}$ ⇒ simultaneous diagonalizable

⇒ have same eigenspace...

By convention, we pick L_z to be the component that we work with...

☑ Want to find functions f where $\{L^2 f = \lambda f, \; L_z f = \mu f\}$

To do this, need angular momentum ladder operators...

$$\boxed{L_\pm = L_x \pm iL_y} \rightsquigarrow \text{for } L_z.$$

Look at more commutators... → $\boxed{[L_z, L_\pm] = \pm\hbar L_\pm}$

$$[L_z, L_\pm] = [L_z, L_x \pm iL_y]$$

$$= [L_z, L_x] \pm i[L_z, L_y] = \dots = \pm\hbar L_\pm$$

Since $L^2 \leftrightarrow L_{z,y,x} \Rightarrow \boxed{[L^2, L_\pm] = 0}$

Suppose

Show ~~iff~~ f is eigenfn of L^2, we also have f eigenfn of L.

- Suppose $L^2 f = \lambda f$. → Since $L^2 \leftrightarrow L_\pm$

  Then $L^2(L_\pm f) = L_\pm(L^2 f) = L_\pm(\lambda f) = \lambda L_\pm f$

  So $\boxed{L_\pm f \text{ is an eigenfn of } L^2\text{, associated w/ } \lambda.}$

- Doing the same trick with L_z...

$$L_z(L_\pm f) = [(L_\pm L_z - L_\pm L_z + L_z L_\pm) f]$$
$$= (L_\pm L_z f) + [L_z, L_\pm] f$$
$$= L_\pm L_z f + (\pm\hbar) L_\pm f$$
$$= (\pm\hbar L_\pm f) + \mu L_\pm f$$

So $\boxed{L_z(L_\pm f) = (\hbar + \mu) L_\pm f}$

So $L_\pm f$ also an eigenfn of L_z, with e-val $(\hbar + \mu)$

↳ $L_\pm$ moves up/down eigenvalue by an $\pm\hbar$ angular momentum

$$L_\pm \longrightarrow \pm\hbar$$

□

Finally, need to terminate... i.e. define top/bottom state...

Define top state ... $\boxed{L_+ f_{top} = 0}$ → give it e-val

$$\boxed{L_z f_{top} = \hbar \overset{m}{\ell} f_z \quad , \quad L^2 f = \lambda f} \rightarrow$$ suppose f is a common eigenvector ...

Rewrite L^2 in terms of ladder op... what

$$L_\pm L_\mp = (L_x \pm i L_y)(L_x \mp i L_y)$$

$$= L_x^2 + L_y^2 \mp i \underbrace{[L_x, L_y]}_{i\hbar L_z}$$

$$= L_x^2 + L_y^2 \pm \hbar L_z$$

$$= \underbrace{L_x^2 + L_y^2} \pm \hbar L_z$$

$$= L^2 - L_z^2 \pm \hbar L_z$$

So... $\boxed{L^2 = L_\pm L_\mp + L_z^2 \mp \hbar L_z}$

Let L^2 act on top state like...

$$L^2 f_{top} = (L_- L_+ + L_z^2 + \hbar L_z) f_{top}$$

$$= L_- \underbrace{L_+ f_{top}} + L_z^2 f_{top} + \hbar L_z f_{top}$$

$$= 0 + (\hbar \ell)^2 f_{top} + (\hbar \ell) f_{top}$$

$$= \hbar^2 \ell(\ell+1) f_{top}$$

$$= \lambda f_{top}$$

So $\boxed{\lambda = \hbar^2 (\ell)(\ell+1)}$

$$\hookrightarrow \boxed{L^2 f_{top} = \hbar^2 \ell(\ell+1) f_{top}}$$

ct 17, 2019

Recall... L^2, L_z share same eigen functions... $L^2 f = \lambda f$

$L_z f = \mu f$

$L_\pm = L_x \pm i L_y$, $[L^2, L_\pm] = 0$, $[L_z, L_\pm] = \pm\hbar L_\pm$

$L^2 = L_\pm L_\mp + L_z^2 \mp \hbar L_z$.

For top state f_t , $\lambda = \hbar^2 \ell(\ell+1)$

Bottom state $f_b \Rightarrow L_- f_b = 0$

Suppose ~~[illegible]~~ $\boxed{L_z f_b = \hbar\bar{\ell} f_b , \quad L^2 f_b = \lambda f_b.}$ → suppose this is true, then

well...

$$L^2 f_b = (L_+L_- + L_z^2 - \hbar L_z) f_b$$

$$= 0 + L_z^2 f_b - \hbar L_z f_b$$

$$= \hbar^2 \bar{\ell}^2 f_b - \hbar^2 f_b$$

$$= \hbar^2 \bar{\ell}(\bar{\ell}-1) f_b.$$

Since eigenvalues for L^2 are the same, $\ell(\ell+1) = \bar{\ell}(\bar{\ell}-1)$

So either $\bar{\ell} = \ell + 1$ (makes no sense since $\bar{\ell}$ lower)

or $\bar{\ell} = -\ell$

$$\boxed{\text{Eigenvalues of } L_z \text{ are } m\hbar \text{ where } -\ell \le m \le \ell , \ m \in \mathbb{Z}}$$

If we have N integer steps $\ell = -\ell + N \rightarrow \ell = \frac{N}{2}$

ℓ is integer or half-integers $\ell = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$

$m = -\ell \ldots 0, \ldots \ell$

⇒ For a given ℓ, there are $(2\ell - 1)$ rungs

$$\boxed{L^2 f_\ell^m = \hbar^2 \ell(\ell+1) f_\ell^m \quad ; \quad L_z f_\ell^m = \hbar m f_\ell^m}$$

Max L value is $\sqrt{\hbar^2 \ell(\ell+1)}$

Max L_z value is $\hbar\ell$

$$\boxed{\hbar\sqrt{\ell(\ell+1)} \geq \hbar\ell}$$

Except for when $\ell = 0$, Uncertainty tells us we can't simultaneously know L_z, L_x, L_y → can't orient so that $L = L_z$ unless $\ell = 0$.

☑ Find eigenfunctions of L^2...

Recall... $\hat{L} = -i\hbar(\vec{r}\times\vec{\nabla})$, $p = -i\hbar\vec{\nabla}$, $\vec{r} = r\hat{r}$

In spherical coordinates... ~~$\vec{\nabla} =$~~

$$\boxed{\vec{\nabla} = \hat{r}\partial_r + \hat{\theta}\frac{1}{r}\partial_\theta + \hat{\phi}\frac{1}{r\sin\theta}\partial_\phi}$$

So,
$$\hat{L} = (-i\hbar)\left\{\underbrace{r(\hat{r}\times\hat{r})\partial_r}_{\vec{0}} + (\hat{r}\times\hat{\theta})\partial_\theta + \frac{1}{\sin\theta}(\hat{r}\times\hat{\phi})\partial_\phi\right\}$$

$$= (-i\hbar)\left\{\hat{\phi}\partial_\theta + \frac{-1}{\sin\theta}\hat{\theta}\partial_\phi\right\}$$

So
$$\boxed{\hat{L} = (-i\hbar)\left\{\hat{\phi}\partial_\theta - \hat{\theta}\frac{1}{\sin\theta}\partial_\phi\right\}}$$

Cartesian:
$$\begin{cases}\hat{\theta} = \cos\theta\cos\phi\,\hat{i} + (\cos\theta\sin\phi)\hat{j} - \sin\theta\,\hat{k} \\ \hat{\phi} = -\sin\phi\,\hat{i} + \cos\phi\,\hat{j}\end{cases}$$

So
$$\boxed{\hat{L} = (-i\hbar)\left\{(-\sin\phi\,\hat{i} + \cos\phi\,\hat{j})\,\partial_\theta - (\cos\theta\cos\phi\,\hat{i} + \cos\theta\sin\phi\,\hat{j} - \sin\theta\,\hat{k})\frac{1}{\sin\theta}\partial_\phi\right\}}$$

And so...

$$\boxed{\begin{aligned} L_x &= (-i\hbar)\left\{-\sin\phi\,\partial_\theta - \cos\phi\cot\theta\,\partial_\phi\right\} \\ L_y &= (-i\hbar)\left\{\cos\phi\,\partial_\theta - \sin\phi\cot\theta\,\partial_\phi\right\} \\ L_z &= (-i\hbar)\,\partial_\phi \\ L_\pm &= L_x \pm iL_y = \dots = \pm\hbar e^{i\phi}\left(\partial_\theta \pm i\cot\theta\,\partial_\phi\right) \end{aligned}}$$

What about L^2? well... $\vec{L} = (-i\hbar)(\vec{r}\times\vec{\nabla})$

and $L^2 = L_\pm L_\mp + L_z^2 - \hbar L_z$

$$= -\hbar^2\left(\partial_\theta^2 + \cot(\theta)\partial_\theta + \cot^2\theta\,\partial_\phi^2 + i\partial_\phi\right)$$

$$= \dots$$

$$\boxed{L^2 = -\hbar^2\left(\frac{1}{\sin\theta}\partial_\theta(\sin\theta\,\partial_\theta) + \frac{1}{\sin^2\theta}\partial\phi^2\right)}$$

We solved this to get Y_ℓ^m...

So $L^2 f_\ell^m = \hbar^2\ell(\ell+1) f_\ell^m$ ← solutions are Y_ℓ^m

$L_z f_\ell^m = -i\hbar\partial_\phi f_\ell^m = m\hbar f_\ell^m$ ← solution are $\Phi(\phi)$

We know Y_ℓ^m are part of the eigenfunctions of $\hat{H}$ for Hydrogen...

This means $\Psi = R(r)\,Y_\ell^m$ are also eigenfunctions of L^2, L_z.

$$\boxed{\hat{H}\Psi = E\Psi, \quad L^2\Psi = \hbar^2 \ell(\ell+1)\Psi, \quad L_z\Psi = \hbar m\Psi}$$

{ Orbital angular momentum only allows integer ℓ }
{ Half-integers are important for spin... }

—//—

SPIN

Model after orbital angular momentum...

Eigenstates get two (eig-val) → $|s m_s\rangle$

↑ need abstract vectors bcz can't write a functional form..

Operators... S^2, S_z .. Same commutation relations...

$$\boxed{\begin{array}{ll} [S_x, S_y] = i\hbar S_z & [S_z, S_x] = i\hbar S_y \\ [S_y, S_z] = i\hbar S_x & S^2|s m_s\rangle = \hbar^2 s(s+1)|s m_s\rangle \\ \multicolumn{2}{c}{S_z|s m_s\rangle = \hbar s\,|s m_s\rangle} \end{array}}$$

Ladder operators... $S_\pm = S_x \pm iS_y$

$$\boxed{S_\pm|s m_s\rangle = \hbar\sqrt{s(s+1) - m(m\pm 1)}\;|s\,(m_s \pm 1)\rangle}$$

Note { eigenstates are NOT spherical harmonics.
Actually not functions at all.
And allow half-int s... $s = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$ $-s \le m \le s$. }

Note: Spin does not change ($s =$ constant) for constant particle

Spin 0: mesons, Higgs boson
Spin $\frac{1}{2}$: p, n, e^-, quarks, ν
Spin 1: photons, gluons
Spin $\frac{3}{2}$: Δ baryons
Spin 2: graviton?

Half-integers → Fermions
Integer → Bosons

Oct 23, 2019

Spin 1/2

Two possible states...

$$s = \frac{1}{2}, \quad m = +\frac{1}{2} \rightarrow \left|\frac{1}{2}\,\frac{1}{2}\right\rangle \text{ or } |\uparrow\rangle \quad \text{(up)}$$

$$s = \frac{1}{2}, \quad m = -\frac{1}{2} \rightarrow \left|\frac{1}{2}\,\frac{-1}{2}\right\rangle \text{ or } |\downarrow\rangle \quad \text{(down)}$$

Can also write as spinors...

$$\boxed{\chi_+ = \begin{pmatrix}1\\0\end{pmatrix} \text{ spin up}, \quad \chi_- = \begin{pmatrix}0\\1\end{pmatrix} \text{ spin down}}$$

General state.

$$\boxed{\chi = a\chi_+ + b\chi_-}$$

Where

$$S^2\chi_+ = \hbar^2 s(s+1)\chi_+ = \frac{3}{4}\hbar^2\chi_+$$

$$S^2\chi_- = \hbar^2 s(s+1)\chi_- = \frac{3}{4}\hbar^2\chi_-$$

What is S^2?

$\Rightarrow \quad S^2 = \begin{pmatrix} c & d \\ e & f \end{pmatrix}$

$$S^2\chi_+ = S^2\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}c\\e\end{pmatrix} = \hbar^2 s(s+1)\begin{pmatrix}1\\0\end{pmatrix} = \frac{3}{4}\hbar^2\begin{pmatrix}1\\0\end{pmatrix}$$

So ~~get~~ $\boxed{S^2 = \frac{3}{4}\hbar^2\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}}$

Do this again to find S_z

$$S_z\chi_+ = +\frac{\hbar}{2}\chi_+ , \quad S_z\chi_- = -\frac{\hbar}{2}\chi_-$$

Let $S_z = \begin{pmatrix}c & d\\e & f\end{pmatrix} \Rightarrow \begin{pmatrix}c\\e\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}1\\0\end{pmatrix} ; \quad \begin{pmatrix}d\\f\end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix}0\\1\end{pmatrix}$

So $\boxed{S_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\0 & -1\end{pmatrix} = \frac{\hbar}{2}\sigma_z}$

Do this one more time for $S_\pm$ ...

~~$S_\pm\chi_\pm = \hbar\chi$, $S_\pm\chi_\mp$~~

$$\boxed{\begin{array}{ll} S_+\chi_- = \hbar\chi_+ , & S_-\chi_- = 0 \\ S_-\chi_+ = \hbar\chi_- , & S_+\chi_+ = 0 \end{array}}$$

When using $\overset{S_\pm, L_\pm}{\wedge}$ normalization it's given by

$$\boxed{\begin{array}{l} S_+ f_\ell^m = \hbar\sqrt{s(s+1) - m(m-1)}\; f_\ell^{m+1} \\ S_- f_\ell^m = \hbar\sqrt{s(s+1) - m(m+1)}\; f_\ell^{m-1} \end{array}}$$

Get $\boxed{S_+ = \hbar\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix} \quad \text{and} \quad S_- = \hbar\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}}$

We also defined $\boxed{S_\pm = S_x \pm iS_y}$

$$S_x = \frac{1}{2}\left(S_+ + S_-\right)$$

$$S_y = \frac{1}{2i}\left(S_+ - S_-\right)$$

$$\boxed{\begin{aligned} S_x &= \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} = \frac{\hbar}{2}\sigma_x \\ S_y &= \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} = \frac{\hbar}{2}\sigma_y \end{aligned}} \quad \text{along with} \quad \boxed{S_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = \frac{\hbar}{2}\sigma_z}$$

In general, write $\boxed{\vec{S} = \frac{\hbar}{2}\vec{\sigma}}$

$$\boxed{\sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad \sigma_y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \quad \sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}}$$

Pauli matrices // Pauli spin matrices. Properties

① $\sigma_x, \sigma_y, \sigma_z, \mathbb{I}_2$ span $\left\{\begin{pmatrix}a & b\\ c & d\end{pmatrix}\right\}$

② $\sigma_x, \sigma_y, \sigma_z, \mathbb{I}_2$ are Hermitian ⇒ real spectrum, $\boxed{\sigma = \sigma^\dagger}$
↳ observables!

③ They are Unitary. $\boxed{\sigma_i\,\sigma_i^\dagger = \sigma_i^\dagger\sigma_i = \mathbb{I}_2}$ $\boxed{\sigma_i^\dagger = \sigma_i^{-1}}$

④ Product of 2 is proportional to the third ...

$\sigma_x\sigma_y = i\sigma_z$, $\sigma_y\sigma_z = \ldots$ $\qquad \boxed{\sigma_i\sigma_j = i\varepsilon_{ijk}\,\sigma_k}$

$\sigma_y\sigma_x = -i\sigma_z$, ...

ε_{ijk}: 1 if (123)

0 if $i=j$... $j=k$.. $k=i$...

-1 if (132)

$\boxed{\sigma_i^2 = \mathbb{I}}$ for $i \neq j$

④ Better ... $\boxed{\sigma_i \sigma_j = \delta_{ij} \mathbb{I} + i \varepsilon_{ijk} \sigma_k}$

⑤ Easy commutation relations...

$$[\sigma_i, \sigma_j] = \sigma_i \sigma_j - \sigma_j \sigma_i$$

$$= i\varepsilon_{ijk}\sigma_k - i\varepsilon_{jik}\sigma_k \quad , \quad \varepsilon_{ijk} = -\varepsilon_{jik}$$

$$\boxed{[\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k} \rightsquigarrow$$

⑤ Anti-commutator...

$$\{\sigma_i, \sigma_j\} = \sigma_i \sigma_j + \sigma_j \sigma_i$$

$$= i\varepsilon_{ijk}\sigma_k + i\varepsilon_{jik}\sigma_k + 2\delta_{ij}\mathbb{I} \quad , \quad \varepsilon_{ijk} = -\varepsilon_{jik}$$

$\boxed{\{\sigma_i, \sigma_j\} = 0}$ for $i \neq j$;

$\boxed{\{\sigma_i, \sigma_j\} = 2\mathbb{I}}$ for $i = j$.

$$\boxed{\{\sigma_i, \sigma_j\} = 2\delta_{ij}\mathbb{I}}$$

$\boxed{\text{Ex}}$ Eigenstates of S_z are χ_+, χ_- by defn.
$(+\frac{\hbar}{2})$, $(-\frac{\hbar}{2})$

What about S_x? $S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & +1 \\ 1 & 0 \end{pmatrix} \rightarrow$ eigenvalues $= \frac{\hbar}{2}, -\frac{\hbar}{2}$

Same for S_y... $S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \rightarrow$ eigenvalues $= \frac{\hbar}{2}, \frac{-\hbar}{2}$

Eigenspinors $\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \pm\frac{\hbar}{2}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \rightarrow \begin{pmatrix} \beta \\ \alpha \end{pmatrix} = \pm\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$

So $\chi_+^{(x)} = A\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \chi_-^{(x)} = B\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

Then, normalize $\Rightarrow$

$$\boxed{\underbrace{\chi_+^{(x)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}}_{\text{eigenvalue } \frac{+\hbar}{2}}, \quad \underbrace{\chi_-^{(x)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}}_{\text{eigenvalue } -\hbar/2}}$$

We can write our general state in terms of $\chi_\pm^{(x)}$

Ex $\chi = \frac{1}{\sqrt{6}}\begin{pmatrix} 1+i \\ 2 \end{pmatrix}$. Want to find $P(+\frac{\hbar}{2})$ for S_z, S_x and $\langle S_x \rangle$.

$$\chi = \frac{1}{\sqrt{6}}\begin{pmatrix} 1+i \\ 2 \end{pmatrix} = \frac{1+i}{\sqrt{6}}\chi_+ + \frac{1}{2\sqrt{6}}\chi_-$$

So $P\left(\frac{+\hbar}{2}, S_z\right) = \left|\frac{1+i}{\sqrt{6}}\right|^2 = \frac{2}{6} = \frac{1}{3}$.

To get (c_+) for $\chi_+^{(x)} \rightarrow$ need to project onto $\chi_+^{(x)}$.

$$\hookrightarrow (c_+) = \chi_+^{\dagger(x)}\chi = \frac{1}{\sqrt{2}}(1 \;\; 1)\left\{\frac{1}{\sqrt{6}}\begin{pmatrix} 1+i \\ 2 \end{pmatrix}\right\}$$

$$= \frac{1}{3\sqrt{2}}\left\{1+i+2\right\} = \frac{3+i}{3\sqrt{2}}.$$

So $\boxed{P\left(\frac{+\hbar}{2}, S_x\right) = \left|\frac{3+i}{3\sqrt{2}}\right|^2 = \frac{\sqrt{10}}{12} = \frac{\sqrt{10}}{12}\,\boxed{\frac{5}{6}}}$

In general, $\boxed{c_\pm^{(i)} = \chi_\pm^{(i)\dagger}\chi}$

$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

$$\boxed{\langle S_x \rangle = \chi^\dagger S_x \chi} = \frac{1}{6}\begin{pmatrix}1-i & 2\end{pmatrix}\frac{\hbar}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}1+i\\2\end{pmatrix}$$

$$= \cdots = \cdots \frac{\hbar}{12}\begin{pmatrix}1-i & 2\end{pmatrix}\begin{pmatrix}2\\1+i\end{pmatrix} = \boxed{\frac{\hbar}{3}\ ?}$$

Oct 24, 2019

ADDING SPIN & ANGULAR MOMENTUM

Two particle system (1) $|s_1 m_1\rangle$

(2) $|s_2 m_2\rangle$

↳ composite state $|s_1 s_2 m_1 m_2\rangle$

Both particles have an S^2 & S_z operator...

$$\overset{|\rangle}{S^{(1)^2}} = \hbar^2 s_1(s_1+1)|s_1 s_2 m_1 m_2\rangle$$

$$|\rangle\ S^{(2)^2} = \hbar^2 s_2(s_2+1)|s_1 s_2 m_1 m_2\rangle$$

$$S_z^{(1)}|\rangle = \hbar m_1|s_1 s_2 m_1 m_2\rangle$$

$$S_z^{(2)}|\rangle = \hbar m_2|s_1 s_2 m_1 m_2\rangle$$

System?

Let total angular momentum

$$\boxed{\vec{S} = \vec{S}^{(1)} + \vec{S}^{(2)}}$$

Finding $S_z = S_z^{(1)} + S_z^{(2)}$

$$\boxed{S_z|s_1 s_2 m_1 m_2\rangle = \hbar\underbrace{(m_1+m_2)}_{m}|s_1 s_2 m_1 m_2\rangle}$$

Trickier with S... Look at two spin 1/2 particles...

↳ Use $|\uparrow\rangle$, $|\downarrow\rangle$ notation...

$S(|a\rangle\otimes|b\rangle)$

$S|a\rangle\otimes S|b\rangle$

$|a\rangle\otimes|b\rangle$

Possible states: $|\uparrow\uparrow\rangle = |\tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}\rangle \quad m = 1$

$$|\uparrow\downarrow\rangle = |\tfrac{1}{2}\ \tfrac{1}{2}\ -\tfrac{1}{2}\ -\tfrac{1}{2}\rangle \quad m = 0$$

$$|\downarrow\uparrow\rangle = |\tfrac{-1}{2}\ \tfrac{-1}{2}\ \tfrac{1}{2}\ \tfrac{1}{2}\rangle \quad m = 0$$

$$|\downarrow\downarrow\rangle = |\tfrac{-1}{2}\ \tfrac{-1}{2}\ \tfrac{-1}{2}\ \tfrac{-1}{2}\rangle \quad m = -1$$

We know that $-s \leq m \leq s$ and moves in integer steps...
But we get two $m=0$ states ⇒ not a good basis...

↳ Start from $|\uparrow\uparrow\rangle$ and apply $S_- = S_-^{(1)} + S_-^{(2)}$

$$S_-|\uparrow\uparrow\rangle = S_-^{(1)}|\uparrow\uparrow\rangle + S_-^{(2)}|\uparrow\uparrow\rangle \qquad (m=1,\ s=1)$$

$$= \hbar|\downarrow\uparrow\rangle + \hbar|\uparrow\downarrow\rangle$$

So $m=0$ state is proportional to $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$ $(s=1)$

Apply S_- again... $S_-\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) = S_-^{(1)}|\uparrow\downarrow\rangle + \cancelto{0}{S_-^{(2)}|\downarrow\uparrow\rangle}$
$+ S_-^{(2)}|\uparrow\downarrow\rangle + \cancelto{0}{S_-^{(2)}|\downarrow\uparrow\rangle}$

So, $S_-\left(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle\right) = 2\hbar|\downarrow\downarrow\rangle$

After normalizing..

$$\boxed{\begin{aligned} &|\uparrow\uparrow\rangle && m=1,\ s=1 \\ &\frac{1}{\sqrt{2}}\left(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle\right) && m=0,\ s=1 \\ &|\downarrow\downarrow\rangle && m=-1,\ s=1 \end{aligned}}$$

triplet states...

Singlet state.

We can also write another state $\boxed{\frac{1}{\sqrt{2}}\left(|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle\right) \quad m=0,\ s=0}$

Check that these have the right S^2 value...

triplet $\rightarrow$ $\hbar\, s(s+1) = 2\hbar$

singlet $\rightarrow$ $\hbar\, s(s+1) = 0\hbar$

Check singlet state $S^2 \frac{1}{\sqrt{2}}\left(|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle\right) = ?$

what is S^2? well...

$$S^2 = \vec{S}\cdot\vec{S} = \left(\vec{S}^{(1)} + \vec{S}^{(2)}\right)^2 =$$

$$= \left(\vec{S}^{(1)} + \vec{S}^{(2)}\right)\cdot\left(\vec{S}^{(1)} + \vec{S}^{(2)}\right)$$

$$\Rightarrow \boxed{S^2 = \vec{S}^{(1)2} + \vec{S}^{(2)2} + 2\vec{S}^{(1)}\cdot\vec{S}^{(2)}}$$

Can write $\boxed{\vec{S}^{(1)}\cdot\vec{S}^{(2)} = S_x^{(1)}S_x^{(2)} + S_y^{(1)}S_y^{(2)} + S_z^{(1)}S_z^{(2)}}$

Next, need to $S_x|\uparrow\rangle \quad S_y|\uparrow\rangle$

$S_x|\downarrow\rangle \quad S_y|\downarrow\rangle$

For example $S_x = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$

so

$$\begin{cases} S_x|\uparrow\rangle = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}1\\ 0\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}0\\ 1\end{pmatrix} = \frac{\hbar}{2}|\downarrow\rangle \\ S_x|\downarrow\rangle = \dots = \frac{\hbar}{2}|\uparrow\rangle \\ S_y|\uparrow\rangle = \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}1\\ 0\end{pmatrix} = \frac{\hbar i}{2}|\downarrow\rangle \\ S_y|\downarrow\rangle = \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}0\\ 1\end{pmatrix} = \frac{-i\hbar}{2}|\uparrow\rangle \end{cases}$$

$\left(S_z|\uparrow\rangle = \frac{\hbar}{2}|\uparrow\rangle \;\; \vdots\right)$

so $\vec{S}^{(1)}\cdot\vec{S}^{(2)}|\uparrow\downarrow\rangle = \underbrace{S_x^{(1)}S_x^{(2)}} + S_y^{(1)}S_y^{(2)} + S_z^{(1)}S_z^{(2)}\;|\uparrow\downarrow\rangle$

$$= \left(\frac{\hbar}{2}\right)^2|\downarrow\uparrow\rangle + \left(\frac{i\hbar}{2}\right)\left(\frac{-i\hbar}{2}\right)|\downarrow\uparrow\rangle + \left(\frac{\hbar}{2}\right)\left(\frac{-\hbar}{2}\right)|\uparrow\downarrow\rangle$$

So $\boxed{\vec{S}^{(1)}\cdot\vec{S}^{(2)}\,|\uparrow\downarrow\rangle = \frac{\hbar^2}{4}\left(2|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle\right)}$

Similarly ; $\vec{S}^{(1)}\cdot\vec{S}^{(2)}\,|\downarrow\uparrow\rangle = \overset{x}{\left(\frac{\hbar}{2}\right)^2|\uparrow\downarrow\rangle} + \overset{y}{\left(\frac{-i\hbar}{2}\right)\left(\frac{i\hbar}{2}\right)|\uparrow\downarrow\rangle} + \overset{z}{\left(\frac{\hbar}{2}\right)\left(\frac{-\hbar}{2}\right)|\downarrow\uparrow\rangle}$

$= \frac{\hbar^2}{4}\left(2|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$

So $\boxed{\vec{S}^{(1)}\cdot\vec{S}^{(2)}\,|\downarrow\uparrow\rangle = \frac{\hbar^2}{4}\left(2|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)}$

eigenstates...

And... $S^{(1)^2}|\uparrow\rangle = S^{(1)^2}|\downarrow\rangle = \hbar^2\frac{1}{2}\left(\frac{1}{2}+1\right)\,|\uparrow\rangle$ or $|\downarrow\rangle$

$= \frac{3}{4}\hbar^2$ and so on...

So $S^2|\downarrow\uparrow\rangle = \frac{3}{4}\hbar^2|\downarrow\uparrow\rangle + \frac{3}{4}\hbar^2|\downarrow\uparrow\rangle + 2\cdot\frac{\hbar^2}{4}\left(2|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$

And

~~$S^2\left\{\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)\right\} = 2\cdot\frac{3\hbar^2}{4}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) + \frac{2}{\sqrt{2}}\cdot\frac{3\hbar^2}{4}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$~~

$\swarrow$

$S^2\left\{\frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right\} = 2\left\{\frac{3\hbar^2}{4}\left(\frac{1}{\sqrt{2}}\left(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle\right)\right)\right\}$

$+ \cancel{\hbar^2}\;2\cdot\frac{1}{\sqrt{2}}\frac{\hbar^2}{4}\left(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle\right)$

$\boxed{S^2\,(+) = 2\hbar^2\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)} \rightsquigarrow (s=1,\ m=0)$

$s(s+1) = 2$

Similarly ... $S^2\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) = 2\cdot\frac{3\hbar^2}{4}\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$

$+2\cdot\frac{3\hbar^2}{4}\frac{1}{\sqrt{2}}\left\{3\left(|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle\right)\right\}$

$\boxed{S^2(-) = 0}$

$s(s+1) = 0$

☑ Two spin $\frac{1}{2}$ particles can have $\boxed{s = \frac{1}{2} + \frac{1}{2} = 1}$

or $\boxed{s = \frac{1}{2} - \frac{1}{2} = 0}$

☑ In general, $\boxed{|s_1 - s_2| \le s \le |s_1 + s_2|}$ integer steps ...

$$\boxed{m = m_1 + m_2}$$

Ex $s_1 = 1, \quad s_2 = \frac{1}{2}, \quad s = \frac{1}{2}, \frac{3}{2} \ldots$

☑ In general, for two particle state $|sm\rangle$

$$\boxed{|sm\rangle = \sum_{m_1+m_2=m} C^{s_1 s_2 s}_{m_1 m_2 m} \, |s_1 s_2 m_1 m_2\rangle}$$

or

$$\boxed{|s_1 s_2 m_1 m_2\rangle = \sum_{s} C^{s_1 s_2 s}_{m_1 m_2 m} \, |sm\rangle}$$

Summarize the "hard" way: start with $s = s_1 + s_2$, $m = s$

$|11\rangle$ for 2 spin $1/2$, then apply $S_-|11\rangle$ until you get to $s = s_1 + s_2$, $m = -s$

$S_-|11\rangle \rightarrow |10\rangle \rightarrow |1\,{-1}\rangle$. Then normalize.

Then, go back to $s = s_1 + s_2$, $m = s-1$ state, find orthogonal state with $s' = s_1 + s_2 - 1$, $m = s'$.

Then do again .... normalize ...

$\boxed{\text{OR}}$ Use $\boxed{\text{Clebsch - Gordan table}}$

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How to read $\int^{S}$ Clebsch-Gordan table ...

Ex		3	$\boxed{2}$	1
		0	0	0
+1	-1	1/5		
0	0	3/5		
-1	+1	1/5		

$$|3\,0\rangle = \frac{1}{\sqrt{5}}\left|\overset{s_1}{2}\;\overset{s_2}{1}\;\overset{m_1}{+1}\;\overset{m_2}{-1}\right\rangle + \sqrt{\frac{3}{5}}\left|2\;1\;0\;0\right\rangle + \frac{1}{\sqrt{5}}\left|2\;1\;-1\;1\right\rangle$$

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$$\boxed{\text{SPIN } 1 + \text{SPIN } 1/2}$$

$$\text{Spin } 1 : \quad |s_1 m_1\rangle = \{\,|1\,1\rangle,\ |1\,0\rangle,\ |1\,-1\rangle\,\}$$

$$\text{Spin } \tfrac{1}{2} : \quad |s_2 m_2\rangle = \left\{\left|\tfrac{1}{2}\ \tfrac{1}{2}\right\rangle, \left|\tfrac{1}{2}\ \tfrac{-1}{2}\right\rangle\right\}$$

Total states

total spin ...

$$|s\ m\rangle = \left\{\left|\tfrac{3}{2}\ \tfrac{3}{2}\right\rangle, \left|\tfrac{3}{2}\ \tfrac{1}{2}\right\rangle, \left|\tfrac{3}{2}\ \tfrac{-1}{2}\right\rangle, \left|\tfrac{3}{2}\ \tfrac{-3}{2}\right\rangle\right.$$

$$\left.\left|\tfrac{1}{2}\ \tfrac{+1}{2}\right\rangle, \left|\tfrac{1}{2}\ \tfrac{-1}{2}\right\rangle\right\}$$

Apply $S_- = S_-^{(1)} + S_-^{(2)}$

$$\begin{cases} S_-^{(1)}\,|1\,1\rangle = \hbar\sqrt{s_1(s_1+1) - m_1(m_1-1)}\ |1\,0\rangle = \hbar\sqrt{2}\,|1\,0\rangle \\ S_-^{(1)}\,|1\,0\rangle = \hbar\sqrt{}\ |1\,-1\rangle = \hbar\sqrt{2}\,|1\,-1\rangle \\ S_-^{(1)}\,|1\,-1\rangle = 0 \end{cases}$$

$$S_-^{(2)} \left|\frac{1}{2}\ \frac{1}{2}\right\rangle = \hbar\sqrt{s_2(s_2+1) - m_2(m_2-1)}\ \left|\frac{1}{2}\ \frac{-1}{2}\right\rangle = \hbar\left|\frac{1}{2}\ \frac{-1}{2}\right\rangle$$

$$S_-^{(2)}\left|\frac{1}{2}\ \frac{-1}{2}\right\rangle = 0$$

Remember $m = m_1 + m_2$

$\Rightarrow$ only way to get $m = \frac{+3}{2} \Rightarrow m_1 = 1,\ m_2 = \frac{+1}{2}$.

$$\left|\frac{3}{2}\ \frac{3}{2}\right\rangle = \left|1\ \frac{1}{2}\ 1\ \frac{1}{2}\right\rangle = \left|s_1\ s_2\ m_1\ m_2\right\rangle$$

		3/2
		3/2
1	1/2	1

Next $$S_-\left|\frac{3}{2}\ \frac{3}{2}\right\rangle = \left(S_-^{(1)} + S_-^{(2)}\right)\left|1\ \frac{1}{2}\ 1\ \frac{1}{2}\right\rangle$$

$$= \hbar\left(\sqrt{2}\left|1\ \frac{1}{2}\ 0\ \frac{+1}{2}\right\rangle + \left|1\ \frac{1}{2}\ 1\ \frac{-1}{2}\right\rangle\right)$$

$$\propto \hbar\left|\frac{3}{2}\ \frac{1}{2}\right\rangle$$

Say $$\left|\frac{3}{2}\ \frac{1}{2}\right\rangle = A\sqrt{2}\left|1\ \frac{1}{2}\ 0\ \frac{+1}{2}\right\rangle + A\left|1\ \frac{1}{2}\ 1\ \frac{-1}{2}\right\rangle$$

$$\Rightarrow A = \frac{1}{\sqrt{3}}$$

So $$\left|\frac{3}{2}\ \frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left|1\ \frac{1}{2}\ 0\ \frac{+1}{2}\right\rangle + \frac{1}{\sqrt{3}}\left|1\ \frac{1}{2}\ 1\ \frac{-1}{2}\right\rangle$$

		3/2
		1/2
1	-1/2	1/3
0	+1/2	2/3

$\rightarrow$ square roots implied...

again

Apply $S_-\left|\tfrac{3}{2}\ \tfrac{1}{2}\right\rangle \propto \hbar\left|\tfrac{3}{2}\ \tfrac{-1}{2}\right\rangle$

$$\left(S_-^{(1)} + S_-^{(2)}\right)\left(\frac{\sqrt{2}}{3}\left|1\ \tfrac{1}{2}\ 0\ \tfrac{1}{2}\right\rangle + \frac{1}{\sqrt{3}}\left|1\ \tfrac{1}{2}\ {+1}\ \tfrac{-1}{2}\right\rangle\right)$$

$$= \hbar\sqrt{\frac{2}{3}}\left\{\left|1\ \tfrac{1}{2}\ {-1}\ \tfrac{1}{2}\right\rangle + \left|1\ \tfrac{1}{2}\ 0\ \tfrac{-1}{2}\right\rangle\right\}$$

$$+ \hbar\frac{1}{\sqrt{3}}\left\{\sqrt{2}\left|1\ \tfrac{1}{2}\ 0\ \tfrac{-1}{2}\right\rangle + \underset{0}{\cancel{\left|1\ \tfrac{1}{2}\ 1\ \tfrac{-1}{2}\right\rangle}}\right\}$$

$$\hbar\left|\tfrac{3}{2}\ \tfrac{-1}{2}\right\rangle \propto \hbar\sqrt{\frac{2}{3}}\left|1\ \tfrac{1}{2}\ {-1}\ \tfrac{1}{2}\right\rangle + \hbar 2\sqrt{\frac{2}{3}}\left|1\ \tfrac{1}{2}\ 0\ \tfrac{-1}{2}\right\rangle$$

So $\left|\tfrac{3}{2}\ \tfrac{-1}{2}\right\rangle = \sqrt{2}A\sqrt{\frac{2}{3}}\left|1\ \tfrac{1}{2}\ {-1}\ \tfrac{1}{2}\right\rangle + 2A\sqrt{\frac{2}{3}}\left|1\ \tfrac{1}{2}\ 0\ \tfrac{-1}{2}\right\rangle$

So $1 = A^2\frac{4}{3} + 4A^2\cdot\frac{2}{3} \Rightarrow A^2 = \frac{\cancel{1}}{\cancel{\sqrt{3}}}\ \frac{3}{12} = \frac{1}{4} \Rightarrow A = \frac{1}{2}$

So

$$\boxed{\left|\tfrac{3}{2}\ \tfrac{-1}{2}\right\rangle = \sqrt{\frac{1}{3}}\left|1\ \tfrac{1}{2}\ {-1}\ \tfrac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\left|1\ \tfrac{1}{2}\ 0\ \tfrac{-1}{2}\right\rangle}$$

		3/2
		-1/2
0	-1/2	2/3
-1	1/2	1/3

Again...

$$S_-\left|\tfrac{3}{2}\ \tfrac{-3}{2}\right\rangle \sim \hbar\left|\tfrac{3}{2}\ \tfrac{-3}{2}\right\rangle$$

$$\left(S_-^{(1)} + S_-^{(2)}\right)\left\{\sqrt{\frac{2}{3}}\left|1\ \tfrac{1}{2}\ 0\ \tfrac{-1}{2}\right\rangle + \sqrt{\frac{1}{3}}\left|1\ \tfrac{1}{2}\ {-1}\ \tfrac{1}{2}\right\rangle\right\}$$

$$= \hbar\sqrt{\frac{2}{3}}\left\{\sqrt{2}\left|1\tfrac{1}{2}\ {-1}\ \tfrac{-1}{2}\right\rangle + 0\right\} + \hbar\sqrt{\frac{1}{3}}\left(0 + \left|1\ \tfrac{1}{2}\ {-1}\ \tfrac{-1}{2}\right\rangle\right)$$

So $\quad \left|\frac{3}{2}\ \frac{-3}{2}\right\rangle = \left|1\ \frac{1}{2}\ -1\ \frac{-1}{2}\right\rangle$

	3/2 −3/2
−1 $-\frac{1}{2}$	1

To find the $\left|\frac{1}{2}\ \frac{1}{2}\right\rangle$, use orthogonality... → must be lin. comb of $\left|1\ \frac{1}{2}\ m_1\ m_2\right\rangle$ $\xrightarrow{}$: $\Sigma m \sim \frac{1}{2}$

$$\left\langle \frac{3}{2}\ \frac{1}{2}\middle|\frac{1}{2}\ \frac{1}{2}\right\rangle = 0$$

$$0 = \left\{\sqrt{\frac{2}{3}}\left\langle 1\ \tfrac{1}{2}\ 0\ \tfrac{1}{2}\right| + \sqrt{\frac{1}{3}}\left\langle 1\ \tfrac{1}{2}\ 1\ \tfrac{-1}{2}\right|\right\}$$
$$\cdot\left\{A\left|1\ \tfrac{1}{2}\ 0\ \tfrac{1}{2}\right\rangle + B\left|1\ \tfrac{1}{2}\ 1\ \tfrac{-1}{2}\right\rangle\right\}$$

$$0 = A\sqrt{\frac{2}{3}} + B\sqrt{\frac{1}{3}} \rightarrow A = \frac{1}{\sqrt{2}}B \Rightarrow A = \sqrt{\frac{1}{3}},\ B = -\sqrt{\frac{2}{3}}$$

So
$$\boxed{\left|\frac{1}{2}\ \frac{1}{2}\right\rangle = -\frac{1}{\sqrt{3}}\left|1\ \tfrac{1}{2}\ 0\ \tfrac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\left|1\ \tfrac{1}{2}\ 1\ \tfrac{-1}{2}\right\rangle}$$

Convention → highest m_1 comes (+

So

	1/2 1/2
1 −1/2	2/3
0 1/2	−1/3

Next, $\quad S_-\left|\frac{1}{2}\ \frac{1}{2}\right\rangle \simeq \hbar_1\left|\frac{1}{2}\ \frac{-1}{2}\right\rangle$

$$\left(S_-^{(1)} + S_-^{(2)}\right)\left\{\frac{-1}{\sqrt{3}}\left|1\ \tfrac{1}{2}\ 0\ \tfrac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\left|1\ \tfrac{1}{2}\ 1\ \tfrac{-1}{2}\right\rangle\right\}$$

$$= \hbar\left(\frac{-1}{\sqrt{3}}\right)\left(\sqrt{2}\left|1\ \tfrac{1}{2}\ -1\ \tfrac{1}{2}\right\rangle + \left|1\ \tfrac{1}{2}\ 0\ \tfrac{-1}{2}\right\rangle\right) + \hbar\sqrt{\frac{2}{3}}\left|1\ \tfrac{1}{2}\ 0\ \tfrac{-1}{2}\right\rangle$$

So $\boxed{\left|\frac{1}{2}\ \frac{-1}{2}\right\rangle = \frac{1}{\sqrt{3}}\left|1\ \frac{1}{2}\ 0\ \frac{-1}{2}\right\rangle - \sqrt{\frac{2}{3}}\left|1\ \frac{1}{2}\ -1\ \frac{1}{2}\right\rangle}$

So

	$1/2$ $-1/2$
$0\ \ -1/2$	$1/3$
$-1\ \ 1/2$	$-2/3$

* * *

ct 28, 2014

Ex e^- in Hydrogen... total angular momentum j

$$j = \underset{\substack{\uparrow \\ \text{orbital angular momentum}}}{l} + s \xrightarrow{\quad} \text{spin} \quad \text{or} \quad j = |l-s|$$

* * *

ELECTRON IN MAGNETIC FIELD

→ Electrons are magnetic dipoles (charged + have spin)

Torque from $\vec{B}$: $\boxed{\vec{\tau} = \vec{\mu} \times \vec{B}}$ where $\boxed{\vec{\mu} = \gamma \vec{S}}$ → magnetic moment

γ ← gyromagnetic ratio.

For electron at rest

$$\boxed{H = -\vec{\mu}\cdot\vec{B} = -\gamma\vec{S}\cdot\vec{B}}$$

Let $\vec{B} = B_0 \vec{k}$. Thus

$$H = -\vec{\mu}\cdot\vec{B} = -\gamma\vec{S}\cdot\vec{B} = -\gamma B_0 S_z$$

So $\boxed{H = -\gamma B_0 \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}$ ⇒ same eigenstates as S_z

$$\left\{\begin{array}{l} \chi_+ \rightsquigarrow E_+ = -\gamma B_0 \hbar/2 \\ \chi_- \rightsquigarrow E_- = +\gamma B_0 \hbar/2 \end{array}\right\}$$

aligned

anti-aligned.

Include time-dependence as usual ...

$$\chi(t) = a\,\chi_+ \exp\left[-iE_+ t/\hbar\right] + b\,\chi_- \exp\left[-iE_- t/\hbar\right]$$

We know $\chi_+ = \begin{pmatrix}1\\0\end{pmatrix}$, $\chi_- = \begin{pmatrix}0\\1\end{pmatrix}$

So $$\boxed{\chi(t) = \begin{pmatrix} a\exp(-iE_+t/\hbar) \\ b\exp(-iE_-t/\hbar)\end{pmatrix}}$$ with $\chi(0) = \begin{pmatrix}a\\b\end{pmatrix}$,

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

Let $a = \cos\frac{\alpha}{2}$, $b = \sin\frac{\alpha}{2}$ $\Rightarrow$ $a^2 + b^2 = 1$

α – fixed angle ...

So $$\boxed{\chi(t) = \begin{pmatrix} \cos\alpha/2 \; e^{-iE_+t/\hbar} \\ \sin\alpha/2 \; e^{-iE_-t/\hbar}\end{pmatrix}}$$

<u>What is $\langle S_x\rangle$, $\langle S_y\rangle$, $\langle S_z\rangle$?</u>

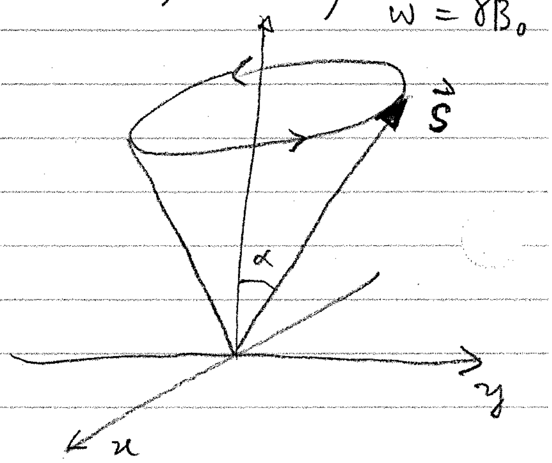
▨ $\langle S_x\rangle = \chi^+ S_x \chi = \frac{\hbar}{2}\sin\alpha\cos(\gamma B_0 t)$

▨ $\langle S_y\rangle = \chi^+ S_y \chi = -\frac{\hbar}{2}\sin\alpha\sin(\gamma B_0 t)$

▨ $\langle S_z\rangle = \chi^+ S_z \chi = \frac{\hbar}{2}\cos(\alpha)$

So
$$\langle \vec{S}\rangle = \frac{\hbar}{2}\left(\sin\alpha\cos(\gamma B_0 t), -\sin\alpha\sin(\gamma B_0 t), +\cos\alpha\right)^T$$

$$\boxed{\langle\vec{S}\rangle = \frac{\hbar}{2}\begin{pmatrix}\sin\alpha\cos(\gamma B_0 t)\\ -\sin\alpha\sin(\gamma B_0 t)\\ \cos\alpha\end{pmatrix}}^{\cancel{T}}$$



↳ Larmor <u>Precession</u> of the expectation values ...

(homogeneous $\vec{B}$)

STERN- GERLACH EXP

Put particles in an inhomogeneous $\vec{B}$. It will experience $\vec{\tau}$, $\vec{F}$

$$\vec{\tau} = \vec{\mu}\times\vec{B} = \text{torque}$$

$$(H = -\vec{\mu}\cdot\vec{B})$$

$$\vec{F} = \vec{\nabla}(\vec{\mu}\cdot\vec{B}) \text{ force}$$

Use neutral particles so no Lorentz force (no $\vec{F} = q\vec{v}\times\vec{B}$)

→ use Silver, Ag.

Let $\boxed{\vec{B} = -\alpha x\,\hat{i} + (B_0 + \alpha z)\,\hat{k}}$

$$\vec{B} = \underbrace{\alpha(-x\hat{i} + z\hat{k})}_{\text{deviation from uniform...}} + \underbrace{B_0\hat{k}}_{\text{strong uniform field}}$$

Since $\vec{\mu} = \gamma\vec{S}$, $\vec{F} = \vec{\nabla}(\vec{\mu}\cdot\vec{B}) = \vec{\nabla}(\gamma\vec{S}\cdot\vec{B})$

$$= \vec{\nabla}\left(-\alpha x\gamma S_x + (B_0 + \alpha z)\gamma S_z\right)$$

$$= -\alpha\gamma S_x\,\hat{i} + \alpha\gamma S_z\,\hat{k}$$

<u>So</u> $\boxed{\vec{F} = -\alpha\gamma(S_x\hat{i} - S_z\hat{k})}$

<u>Know</u> B_0 piece causes precession of S_x, S_y (Larmor)

↳ $\langle S_x\rangle$ will oscillate with freq $\omega = \gamma B_0$. If B_0 very large, this precession will be very fast

→ average to zero...

→ $\vec{F}$ becomes only in z-direction → $\boxed{\vec{F} = \alpha\gamma S_z\hat{k}}$

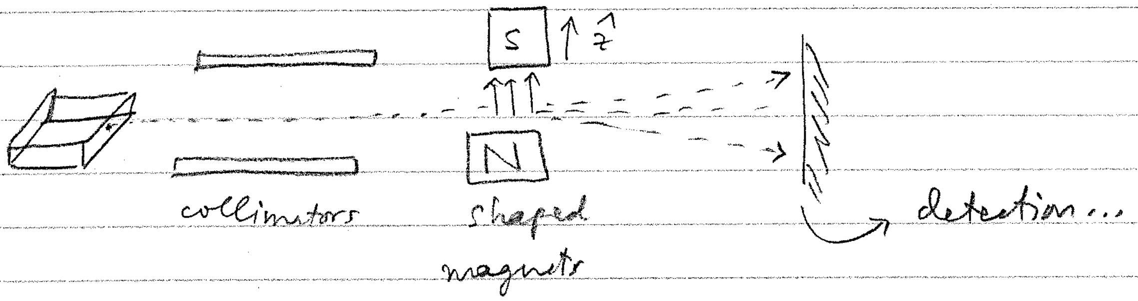
☒ Particle passing through $\vec{B}$ field feel force proportional to S_z. For spin $\frac{1}{2}$ → ↑ deflected up.

↳ ↓ deflected down.

☒ For higher spin → get $2s+1$ m values ⇒ $2s+1$ beams.

☒ Stern-Gerlach used silver atoms → one unpaired electron

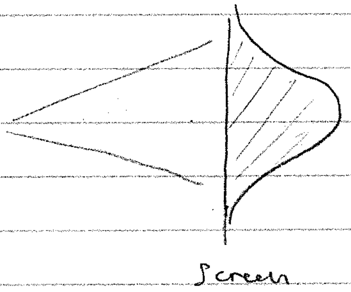
⟹ spin 1/2.



Particles heated in oven, pass through collimator, then $\vec{B}$ field. Atoms in initial beam are unpolarized → no preferred direction for magnetic moment $\vec{\mu}$

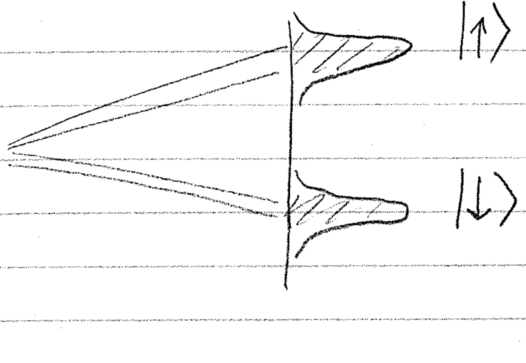
Classically, μ_z can range continuously from $+\mu$ to $-\mu$

↳ expect



since μ_z can be anything from $-\mu$ to $+\mu$

But what happened ... spin is quantized. μ_z only has 2 values ..



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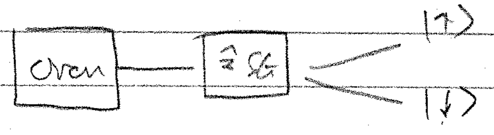


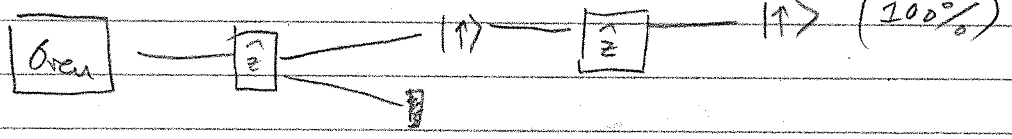
Send through SG $\hat{z}$

→ say definitely it we have

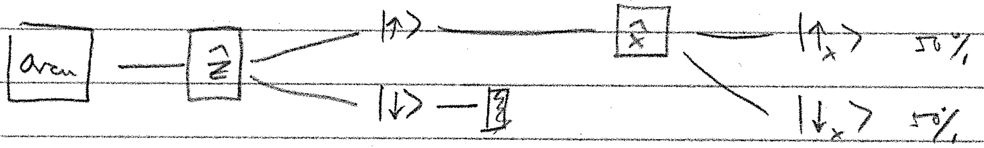
$|\uparrow\rangle$ or $|\downarrow\rangle$ wrt $\hat{z}$

(1/2) (1/2) 50~50

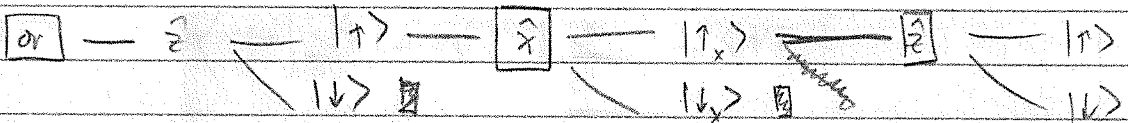
- Run through $\hat{z}$ again, $|\uparrow\rangle$ only



- What if second stage is $\hat{x}$? $\rightsquigarrow$ $|\uparrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow_x\rangle + |\downarrow_x\rangle)$



- Put a 3rd SG $\hat{z}$ ...



Since $|\uparrow_x\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$

—//—

Eigenvalue problem: eigenvalues det$|A - \lambda \mathbb{I}| = 0$

$$A = \begin{pmatrix} 1 & 1 & 0 \\ -1 & 2 & -1 \\ 0 & 1 & 1 \end{pmatrix} \rightsquigarrow \lambda = 0, 1, 3$$

$$\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \quad \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \quad \begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}$$

$B = PAP^{-1}$, $P^{-1} = \begin{pmatrix} \text{matrix of} \\ \text{eigenvec} \end{pmatrix}$

Eigenvector B is $\{e_1, e_2, e_3\}$

$$= \begin{pmatrix} 3 & & \\ & 1 & \\ & & 0 \end{pmatrix}$$

Ex 4.64 H in state $\psi = R_{21}\left(\sqrt{\frac{1}{3}}\,Y_1^0\chi_+ + \sqrt{\frac{2}{3}}\,Y_1^1\chi_-\right)$

let $|n\ l\ m_\ell\ m_s\rangle$

$$|\psi\rangle = \frac{1}{\sqrt{3}}\,|2\ 1\ \underbrace{0\ \tfrac{+1}{2}}_{m_\ell\ m_s}\rangle + \frac{\sqrt{2}}{\sqrt{3}}\,|2\ 1\ \underbrace{1\ \tfrac{-1}{2}}_{m_\ell\ m_s}\rangle$$

orbital angular momentum $L^2|\psi\rangle = \hbar^2(\ell+1)\ell\,|\psi\rangle = 2\hbar^2|\psi\rangle$

$$L_z|\psi\rangle \sim \frac{1}{\sqrt{3}}|0\rangle + \frac{\sqrt{2}}{\sqrt{3}}|1\rangle \longrightarrow \frac{1}{3} \text{ in } 0\hbar$$

$\frac{2}{3}$ in $\hbar$

$$S^2|\psi\rangle = \frac{3}{4}\hbar^2|\psi\rangle$$

$$S_z|\psi\rangle \sim \frac{1}{\sqrt{3}}\left|+\tfrac{1}{2}\right\rangle + \frac{\sqrt{2}}{\sqrt{3}}\left|-\tfrac{1}{2}\right\rangle$$

Total… $j = \ell + s = \frac{3}{2}$ $\frac{1}{2}$

or $j = \ell - s = \frac{1}{2}$

$\longrightarrow$ $|\ell\ s\ m_\ell\ m_s\rangle$

$$J^2|\psi\rangle = \hbar^2 j(j+1)|\psi\rangle \quad \left\{ \psi = \frac{1}{\sqrt{3}}\left|1\ \tfrac{1}{2}\ 0\ \tfrac{+1}{2}\right\rangle + \sqrt{\frac{2}{3}}\left|1\ \tfrac{1}{2}\ 1\ \tfrac{-1}{2}\right\rangle \right.$$

Rewrite $|2\,1\,0\,\tfrac{+1}{2}\rangle$ in $|j\,m_j\rangle$

$$\left|\underset{s_1}{1}\ \underset{s_2}{\tfrac{1}{2}}\ \underset{m_{s_1}}{0}\ \underset{m_{s_2}}{\tfrac{+1}{2}}\right\rangle = \sqrt{\frac{2}{3}}\left|\overset{j}{\tfrac{3}{2}}\ \overset{m_j}{\tfrac{1}{2}}\right\rangle - \frac{1}{\sqrt{3}}\left|\overset{j}{\tfrac{1}{2}}\ \overset{m_j}{\tfrac{1}{2}}\right\rangle$$

$$\left|1\ \tfrac{1}{2}\ 1\ \tfrac{-1}{2}\right\rangle = \frac{1}{\sqrt{3}}\left|\tfrac{3}{2}\ \tfrac{1}{2}\right\rangle + \frac{\sqrt{2}}{\sqrt{3}}\left|\tfrac{1}{2}\ \tfrac{1}{2}\right\rangle$$

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So $|\psi\rangle = \frac{2\sqrt{2}}{3}\left|\tfrac{3}{2}\ \tfrac{1}{2}\right\rangle + \frac{1}{3}\left|\tfrac{1}{2}\ \tfrac{1}{2}\right\rangle$

So $J^2\psi = j(j+1)\hbar^2\psi = \frac{15}{4}\hbar^2$, $P = 8/9$

$= 3/4\,\hbar^2$, $P = 1/9$

Ex $\boxed{\text{Deuterium — Bound proton + neutron}}$

From exp ~> $j = \underline{1}$.

Both p & n have spin 1/2.

$S_{tot} = s + s \ldots 0 = 0$ or 1.

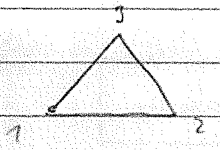
Since $j = 1$, $s = 0, 1 \Rightarrow l = 0$ or 1 or 2

$j = l + S_{tot}$
or $j = |l - S_{tot}|$

$j = 1$ and $S_{tot} = 0$ then $l = \underline{1}$

$j = 1$ & $S_{tot} = 1$ then $l = \underline{0 \text{ or } 2}$

Ex $\boxed{4.67}$ $\boxed{3 \text{ spin } \tfrac{1}{2} \text{ particles arranged in triangle...}}$



$$H = J\left(\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_3 \cdot \vec{S}_1\right)$$

Want to rewrite this in terms of S_1^2, S_2^2, ...

- $\vec{S} = \vec{S}_1 + \vec{S}_2 + \vec{S}_3$ $\qquad [S_i, S_j] = 0$

- $$\vec{S}^2 = \vec{S} \cdot \vec{S} = (\vec{S}_1 + \vec{S}_2 + \vec{S}_3)^2 = \vec{S}_1^{\,2} + \vec{S}_2^{\,2} + \vec{S}_3^{\,2} + 2\left(\vec{S}_1 \cdot \vec{S}_2 + \vec{S}_2 \cdot \vec{S}_3 + \vec{S}_3 \cdot \vec{S}_1\right)$$

So $$H = \frac{J}{2}\left\{ S^2 - \underbrace{S_1^2 - S_2^2 - S_3^2}_{3\left(\frac{3}{4}\hbar^2\right) \rightsquigarrow \text{ spin } 1/2} \right\}$$

S^2? 2 particles + 1 particle

$s = 0$ $\quad s = 1$ $\qquad s = \frac{1}{2}$ $\Rightarrow S = \frac{1}{2}$ or $\frac{3}{2}$

$0 \pm \frac{1}{2} = \frac{1}{2}$, $\left|1 \pm \frac{1}{2}\right| = \frac{1}{2}$ or $\frac{3}{2}$ $\qquad s = \frac{1}{2}$ $\qquad s = \frac{3}{2}$

$$S^2 = \hbar^2 S_{tot}(S_{tot} + 1) = \boxed{\frac{3}{4}\hbar^2 \text{ or } \frac{15}{4}\hbar^2}$$

So possible values for Hamiltonian → ~~$H = E = \frac{J}{2}\left(\frac{3}{4}\hbar^2 - 3\cdot\frac{3}{4}\hbar^2\right)$~~

So $H = \frac{J}{2}\left(\frac{3}{4}\hbar^2 - 3\cdot\frac{3}{4}\hbar^2\right) = -\frac{3}{2}\hbar^2\frac{J}{2} = -\frac{3}{4}\hbar^2 J \quad (s = \frac{1}{2})$

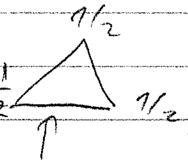
or $H = \frac{J}{2}\left(\frac{15}{4}\hbar^2 - 3\cdot\frac{3}{4}\hbar^2\right) = \frac{6}{8}J\hbar^2 = \frac{3}{4}J\hbar^2 \quad (s = \frac{3}{2})$

→ $S_{tot} = \frac{1}{2}$ is the ground state → degeneracy of 4

↳ $S_{tot} = \underbrace{0 + \frac{1}{2}}_{} = \underbrace{(1 - \frac{1}{2})}_{}$

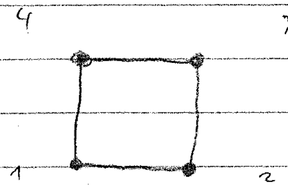
one way to get $s_1 = 0$

degeneracy 1 (degeneracy 3, since



3 ways to get $s_2 = 1$ (3 ways)

Ex $\boxed{\text{4 spin 1/2 particles in a square}}$



$$H = J\left(\vec{S}_1\cdot\vec{S}_2 + \vec{S}_2\cdot\vec{S}_3 + \vec{S}_3\cdot\vec{S}_4 + \vec{S}_4\cdot\vec{S}_1\right)$$

use again: $\vec{S} = \vec{S}_1 + \vec{S}_2 + \vec{S}_3 + \vec{S}_4$
$= (\vec{S}_1 + \vec{S}_3) + (\vec{S}_2 + \vec{S}_4)$

$$S^2 = (\vec{S}_1 + \vec{S}_3)^2 + (\vec{S}_2 + \vec{S}_4)^2 + 2(\vec{S}_1 + \vec{S}_3)(\vec{S}_2 + \vec{S}_4)$$
$$= (\vec{S}_1 + \vec{S}_3)^2 + (\vec{S}_2 + \vec{S}_4)^2 + 2(\ldots\ldots)$$

So $H = \frac{J}{2}\left(S^2 - (\vec{S}_1 + \vec{S}_3)^2 - (\vec{S}_2 + \vec{S}_4)^2\right)$

2 particles + 2 particles
$s = 0, 1$ $\quad$ $s = 0, 1$

	0	1
0	0	1
1	1	2, 0

$S_{tot} = 0, 1, 2 \ldots$

~~[illegible]~~

	~~-1~~	~~0~~	~~1~~
~~-1~~	~~+2~~	~~1~~	~~0~~
~~0~~	~~1~~	~~0~~	~~1~~
~~1~~	~~0~~		~~2~~

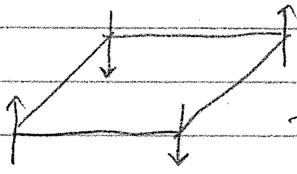
	0	1
0	0	1
1	1	2,0

So $S_{tot} = 0 \rightarrow 2$ ways

$$(0,0) \quad E_0 = \frac{J}{2}\left(\hbar^2 0(0+1) - 0 - 0\right) = \boxed{0}$$

$$(1,1) \quad E_0' = \frac{J}{2}\left(\hbar^2 0(0+1) - \hbar^2 1(1+1) - \hbar^2 1(1+1)\right)$$

$$= \boxed{-2\hbar^2 J} \rightsquigarrow \text{ground state} \ldots$$



⤳ ground state … everything is anti aligned …

CENTRAL POTENTIALS

Review

Nov 7, 2019

Recall $V(r) = V$

$\psi(r, \theta, \varphi) = R(r) Y_m^{\ell}(\theta, \varphi)$

Radial … $\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) - \frac{2m}{\hbar}\left(V(r) - E\right) R = \ell(\ell+1) R$

Usually $u(r) = rR(r)$

$$\frac{-\hbar^2}{2m} \partial_r^2 u + \left(V + \frac{\ell(\ell+1)}{r^2}\right) u = Eu.$$

ANGULAR MOMENTUM

$$[L_i, L_j] = i\hbar\epsilon_{ijk} L_k$$

L^2, H, L_z share eFn $\Rightarrow$ $E\psi = H\psi$

$\hbar^2 \ell(\ell+1)\psi = L^2\psi$

$\hbar m_\ell \psi = L_z \psi$

$L_\pm = L_x \pm iL_y$

$$L_\pm Y_\ell^m = \hbar \sqrt{\ell(\ell+1) - m(m\pm1)} \; Y_\ell^{m\pm1}$$

$\ell = 0, 1, 2, \ldots \qquad -\ell \leq m \leq \ell.$ int step

SPIN

$[S_i, S_j] = i\hbar \varepsilon_{ijk} S_k$

State → $|sm\rangle$ ... $S^2 |sm\rangle = \hbar^2 s(s+1) |sm\rangle$

$S_z |sm\rangle = \hbar m_s |sm\rangle$

$S_\pm = S_x \pm i S_y$

$$S_\pm |sm\rangle = \hbar \sqrt{s(s+1) - m(m\pm1)}\ |s\,m\pm1\rangle$$

$s = 0, 1/2, 1, \ldots$ $\quad -s \le m_s \le s$ int step

ADDING SPIN

$\vec{S} = \vec{S}_1 + \vec{S}_2$ $\quad s = s_1 + s_2$ or $s = |s_2 - s_1|$, int step

$m = m_{s_1} + m_{s_2}$.

Can write combined state $|sm\rangle$ in terms of $|s_1 s_2 m_1 m_2\rangle$ using Clebsch Gordan table or raising – lowering operators..

SPINORS

Spin 1/2 → $\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ → S_z eigenspinors..

$$\underset{\text{prob. amplitude}}{c_\pm} = \underbrace{\chi_\pm^{(x,y)\dagger}}_{\text{whatever state you want to find}} \underbrace{\chi}_{\text{state}}$$

Construct S_x, S_y, S_z by looking at general matrix times eigenspinors and remembering $S_x = \frac{1}{2}(S_+ + S_-)$

$S_y = \frac{1}{2i}(S_+ - S_-)$

Spin (1/2) $\rightarrow$ $S_+|+\rangle = 0$ $\quad \begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

$S_-|-\rangle = 0$ $\quad \begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}\hbar$

S_z eigenspinor ....

GENERAL UNCERTAINTY PRINCIPLE

$$\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i} \left\langle [\hat{A}, \hat{B}] \right\rangle \right)^2$$

GENERAL EHRENFEST

$$\frac{d}{dt}\langle Q \rangle = \frac{i}{\hbar}\left\langle [\hat{Q}, \hat{H}] \right\rangle + \underbrace{\langle \partial_t \hat{Q} \rangle}_{\text{usually } 0}$$

ov 4, 2019

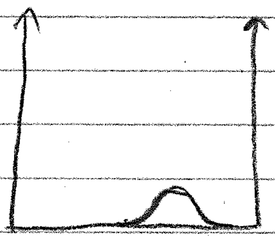
PERTURBATION THEORY

Start with problems you can solve ... (1D ∞ well)

$$\boxed{H^{(0)} \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}}$$

(0): original problem. $\langle \psi_n^{(0)} | H^{(0)} | \psi_n^{(0)} \rangle = E_n^{(0)}$

Add perturbation ...



New H, new ψ_n, new E_n

Can't solve directly ... Instead, let

$$\boxed{H = \underset{\text{original}}{\underset{\uparrow}{H^{(0)}}} + \underset{\text{small, then increase gradually}}{\underset{\uparrow}{\lambda}} \overset{\text{perturbation}}{H'}}$$

Then, $\boxed{\psi_n = \psi_n^{(0)} + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} + \dots}$

Similarly, $\boxed{E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots}$

Superscript (1) ⇒ 1st order correction.
(2) ⇒ 2nd order correction.

New problem

$$(H_0 + \lambda H')(\psi_n^{(0)} + \lambda\psi_n^{(1)} + \lambda^2\psi_n^{(2)} +)$$

$$= (E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)})(\psi_n^{(0)} + \lambda\psi_n^{(1)} + \lambda^2\psi_n$$

Multiply out to get powers of λ ...

$$\left\{\begin{aligned} &H^{(0)}\psi_n^{(0)} + \lambda(H^{(0)}\psi_n^{(1)} + H'\psi_n^{(0)}) + \lambda^2(H^{(0)}\psi_n^{(2)} + H'\psi_n^{(1)}) \\ &= E_n^{(0)}\psi_n^{(0)} + \lambda(E_n^{(0)}\psi_n^{(1)} + E_n^{(1)}\psi_n^{(0)}) \\ &\quad + \lambda^2(E_n^{(2)}\psi_n^{(0)} + E_n^{(1)}\psi_n^{(1)} + E_n^{(0)}\psi_n^{(2} \end{aligned}\right.$$

So lowest order in λ .. $\boxed{H^{(0)}\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)}}$

First order in λ : $\boxed{H^{(0)}\psi_n^{(1)} + H'\psi_n^{(0)} = E_n^{(0)}\psi_n^{(1)} + E_n^{(1)}\psi_n^{(0)}}$

2nd order in λ : $\boxed{H^{(0)}\psi_n^{(2)} + H'\psi_n^{(1)} = E_n^{(0)}\psi_n^{(2)} + E_n^{(1)}\psi_n^{(1)} + E_n^{(2)}\psi_n^{(2}}$

Nov 7, 2019

$$|\psi_n\rangle = |\psi_n^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle + \lambda^2|\psi_n^{(2)}\rangle$$

$\boxed{\lambda^0}$: $H^{(0)}|\psi_n^{(0)}\rangle = E_n^{(0)}\psi_n^{(0)}$

$\boxed{\lambda^1}$ $H^{(0)}|\psi_n^{(1)}\rangle + H|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(1)}\rangle + E_n^{(1)}|\psi_n^{(0)}\rangle$

$\boxed{\lambda^2}$: $H^{(0)}|\psi_n^{(2)}\rangle + H'|\psi_n^{(1)}\rangle = \dots$

<u>Look at 1^{st} order</u> → multiply by $\langle \psi_n^{(0)}|$

$$\langle \psi_n^{(0)}|H^{(0)}|\psi_n^{(1)}\rangle + \langle \psi_n^{(0)}|H'|\psi_n^{(0)}\rangle$$

$$= E_n^{(0)}\langle \psi_n^{(0)}|\psi_n^{(1)}\rangle + E_n^{(1)}\underbrace{\langle \psi_n^{(0)}|\psi_n^{(0)}\rangle}_{1}$$

We know

$$H^{(0)}|\psi_n^{(0)}\rangle = E_n^{(0)}|\psi_n^{(0)}\rangle \rightarrow \langle \psi_n^{(0)}|\underset{\uparrow\ \text{Hermitian...}}{H^{(0)}} = \langle \psi_n^{(0)}|\overset{\in\mathbb{R}.}{E_n^{(0)}}$$

And so

$$\langle \psi_n^{(0)}|H^{(0)}|\psi_n^{(1)}\rangle = E_n^{(0)}\langle \psi_n^{(0)}|\psi_n^{(1)}\rangle$$

So

$$\cancel{E_n^{(0)}\langle \psi_n^{(0)}|\psi_n^{(1)}\rangle} + \langle \psi_n^{(0)}|H'|\psi_n^{(0)}\rangle$$

$$= \cancel{E_n^{(0)}\langle \psi_n^{(0)}|\psi_n^{(1)}\rangle} + E_n^{(1)}$$

So

$$\boxed{E_n^{(1)} = \langle \psi_n^{(0)}|H'|\psi_n^{(0)}\rangle}$$

Ex ∞-square well with delta function in the middle...

$$H^{(0)} = \frac{\hat{p}^2}{2m} + V(x) \qquad V(x) = \begin{cases} 0 & -a \leq x \leq a \\ \infty & |x| > a \end{cases}$$

$$H^{(1)} = H' = \alpha\,\delta(x).$$

We know that the <u>unperturbed</u> solution:

$$|\psi_n^{(0)}\rangle = \begin{cases} \frac{1}{\sqrt{a}}\cos\left(\frac{\pi n x}{2a}\right) & n \text{ odd} \\ \frac{1}{\sqrt{a}}\sin\left(\frac{\pi n x}{a}\right) & n \text{ even} \end{cases}$$

Energies $\boxed{\frac{n^2\pi^2\hbar^2}{2m(2a)^2} = E_n}$

Need to look at first-order correction ...

Ground state $E_1^{(1)} = \langle \psi_1^{(0)} | \alpha \delta(x) | \psi_1^{(0)} \rangle$

$$= \int_{-a}^{a} \psi_1^{*(0)} \alpha \delta(x) \psi_1^{(0)} dx$$

$$= \frac{1}{a} \int_{-a}^{a} \alpha \delta(x) \cos^2\left(\frac{\overset{1}{\cancel{n}}\pi x}{a}\right) dx$$

$$\boxed{E_1^{(1)} = \frac{\alpha}{a}}$$

So, for all n odd → $\boxed{E_n^{(1)} = \frac{\alpha}{a}}$ (even states)

Look at $n = 2$ ... (first excited state)

$$E_2^{(1)} = \langle \psi_2^{(1)} | \alpha \delta(x) | \psi_2^{(1)} \rangle$$

$$= \frac{1}{a} \int_{-a}^{a} \alpha \delta(x) \sin^2\left(\frac{2\pi x}{a}\right) dx = \boxed{0}$$

So for all n even $\boxed{E_n^{(1)} = 0}$ (odd states)

What about corrections to the wavefunction?

First order eqn: $H^{(0)} |\psi_n^{(1)}\rangle + H' |\psi_n^{(0)}\rangle = E_n^{(0)} |\psi_n^{(1)}\rangle + E_n^{(1)} |\psi_n^{(0)}\rangle$

↳ Rearrange: $\boxed{(H^{(0)} - E_n^{(0)}) |\psi_n^{(1)}\rangle = \underbrace{-(H' - E_n^{(1)}) |\psi_n^{(0)}\rangle}_{\text{known ...}}}$

This is a diff. eqn for $|\psi_n^{(1)}\rangle$ ...

↳ write it as combination of unperturbed states ...

$|\psi_n^{(0)}\rangle$ form a complete basis...

$$\boxed{|\psi_n^{(1)}\rangle = \sum_{m\neq n} C_m |\psi_m^{(0)}\rangle}$$ why drop n term?

So... $(H^{(0)} - E_n^{(0)}) \sum'_{m\neq n} C_m |\psi_m^{(0)}\rangle = -(H' - E_n^{(1)})|\psi_n^{(0)}\rangle$

So $\sum'_{m\neq n} (E_m^{(0)} - E_n^{(0)}) C_m |\psi_m^{(0)}\rangle = -(H' - E_n^{(0)})|\psi_n^{(0)}\rangle$

So → Fourier's Trick ... $\langle\psi_l^{(0)}|$

So $\sum'_{m\neq n} C_m \langle\psi_l^{(0)}|(E_m^{(0)} - E_n^{(0)})|\psi_m^{(0)}\rangle = -\langle\psi_l^{(0)}|(H' - E_n^{(0)})|\psi_n^{(0)}\rangle$

$$\sum'_{m\neq n} C_m (E_m^{(0)} - E_n^{(0)}) \underbrace{\langle\psi_l^{(0)}|\psi_m^{(0)}\rangle}_{\delta^l_m} = -\langle\psi_l^{(0)}|H'|\psi_n^{(0)}\rangle + E_n^{(0)} \underbrace{\langle\psi_l^{(0)}|\psi_n^{(0)}\rangle}_{\delta^l_n\text{, but } l=m\neq n}$$

So $\sum'_{m\neq n} C_m (E_m^{(0)} - E_n^{(0)})\, \delta^l_m = -\langle\psi_l^{(0)}|H'|\psi_n^{(0)}\rangle + \underbrace{E_n^{(0)}\delta_{ln}}_{\to 0}$

Get

$$C_l (E_l^{(0)} - E_n^{(0)}) = -\langle\psi_l^{(0)}|H'|\psi_n^{(0)}\rangle$$

Find $$\boxed{C_m = \frac{+\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}}}$$

So, first order correction... $$\boxed{|\psi_n^{(1)}\rangle = \sum_{m\neq n} \frac{\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}}|\psi_m^{(0)}\rangle}$$

↑ This only works for non-degenerate where $E_n^{(0)} = E_m^{(0)} \Leftrightarrow m = n$

→ Must assume non-degenerate solutions

<u>Back to example</u> to find $|\psi_n^{(1)}\rangle$ ... expect 0 for $|\psi_{\text{even}}^{(1)}\rangle$

Well...

ground state →

$$\boxed{|\psi_1^{(1)}\rangle = \sum_{m\neq 1} \frac{\langle\psi_m^{(0)}|\alpha\delta(x)|\psi_1^{(0)}\rangle}{E_1^{(0)}-E_m^{(0)}}|\psi_m^{(0)}\rangle}$$

Look at

$$\langle\psi_m^{(0)}|\alpha\delta(x)|\psi_1^{(0)}\rangle = \begin{cases} \frac{1}{a}\int_{-a}^{a}\alpha\delta(x)\sin\left(\frac{m\pi x}{a}\right)\cos\left(\frac{\pi x}{a}\right)dx, & m \text{ eve} \\ \frac{1}{a}\int_{-a}^{a}\alpha\delta(x)\cos\left(\frac{m\pi x}{a}\right)\cos\left(\frac{\pi x}{a}\right)dx, & m \text{ eve} \end{cases}$$

$$= \begin{cases} 0, & m \text{ even} \\ \frac{\alpha}{a}, & m \text{ odd} \end{cases}$$

Also,

$$\boxed{E_1^{(0)}-E_m^{(0)} = \frac{\pi^2\hbar^2}{2\underset{\uparrow \text{ mass}}{m_e}(2a)^2}(1^2-m^2)}$$

<u>So</u>

$$\boxed{|\psi_\ell^{(1)}\rangle = \sum_{\substack{m\neq \ell \\ m \text{ odd}}}{}' \frac{\alpha}{a}\,\frac{2m_e(2a)^2}{\pi^2\hbar^2(\ell^2-m^2)}|\psi_m^{(0)}\rangle}$$

→ true for all ℓ odd

<u>Note</u> $\boxed{\text{all } \ell \text{ even } |\psi_\ell^{(1)}\rangle = 0.}$

Again, all this works only when non-degenerate ...

Nov 8, 2019

Second-order non-degenerate

$$H^{(0)}|\psi_n^{(2)}\rangle + H'|\psi_n^{(1)}\rangle = E_n^{(2)}|\psi_n^{(0)}\rangle + E_n^{(1)}|\psi_n^{(1)}\rangle + E_n^{(0)}|\psi_n^{(2)}\rangle$$

multiply by $\langle\psi_n^{(0)}|$ and cancel...

$$\langle\psi_n^{(0)}|H'|\psi_n^{(1)}\rangle = E_n^{(2)} + E_n^{(1)}\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle$$

Look at $\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle = \langle\psi_n^{(0)}| \sum_{m\neq n} \underbrace{\frac{\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle}{E_n^{(0)} - E_m^{(0)}}}_{c_m} |\psi_m^{(0)}\rangle$

So $\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle = \sum_{m\neq n} c_m \cancelto{0}{\langle\psi_n^{(0)}|\psi_m^{(0)}\rangle}$ $(m\neq n)$

So $E_n^{(2)} = \langle\psi_n^{(0)}|H'|\psi_n^{(1)}\rangle = \sum_{m\neq n}\langle\psi_n^{(0)}|H'|c_m\psi_m^{(0)}\rangle$

$$\boxed{E_n^{(2)} = \sum_{m\neq n} \frac{|\langle\psi_m^{(0)}|H'|\psi_n^{(0)}\rangle|^2}{E_n^{(0)} - E_m^{(0)}}}$$

Ex 1D SHO + Relativistic correction... $T = \sqrt{m^2c^4 + p^2c^2}$

$$\simeq \frac{p^2}{2m} - \frac{p^4}{8m^3c^2}$$

So $H = \underbrace{\frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2}_{H^{(0)}} - \underbrace{\frac{p^4}{8m^3c^2}}_{H'}$, $|n\rangle$

1^{st} order $E_0^{(1)} = \langle 0|H'|0\rangle$ $\hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}_+ - \hat{a}_-)$

$$E_0^{(1)} = \langle 0|\left(i\sqrt{\frac{\hbar\omega m}{2}}\right)^4\left(\frac{-1}{8m^3c^2}\right)(\hat{a}_+ - \hat{a}_-)^4|0\rangle = \frac{-\hbar^2\omega^2}{32mc^2}\langle 0|\underbrace{(\hat{a}_+ - \hat{a}_-)^4|0\rangle}_{\text{do this}}$$

$$(\hat{a}_+ - \hat{a}_-)^4|0\rangle = (\hat{a}_+ - \hat{a}_-)\sqrt{6}|3\rangle - 3|1\rangle = 2\sqrt{6}|4\rangle - \sqrt{6}\sqrt{3}|2\rangle$$
$$- 3\sqrt{2}|2\rangle + 3|0\rangle$$

So $2\sqrt{6}|4\rangle - 6\sqrt{2}|2\rangle + 3|0\rangle = (\hat{a}_+ - \hat{a}_-)^4|0\rangle$

Take the inner prod to find...

$$\boxed{E_0^{(1)} = \frac{-3\hbar^2 w^2}{32mc^2}}$$

1st order correction to evtrs sum collapse to 2 terms $m=2$, $m=4$.

$$|0^{(1)}\rangle = \frac{\langle 2|H'|0\rangle}{-2\hbar w}|2\rangle + \frac{\langle 4|H'|0\rangle}{-4\hbar w}|4\rangle$$

$$= \dots$$

$$= \frac{-\hbar w}{64mc^2}\left[-\sqrt{6}\,|4\rangle + 6\sqrt{2}\,|2\rangle\right] \longrightarrow \text{not normalized.}$$

Now need $E_0^{(2)}$

$$E_0^{(2)} = \left(\frac{-\hbar^2 w^2}{32mc^2}\right)^2\left[\frac{-1}{4\hbar w}(2\sqrt{6})^2 - \frac{1}{2\hbar w}(-\sqrt{6}\sqrt{2})^2\right.$$

$$= \boxed{\frac{\hbar^3 w^3}{m^2c^4}\left[\frac{1}{32^2}(-8-36)\right]}$$

Full energy to 2nd order

$$E_0 = E_0^{(0)} + E_0^{(1)} + E_0^{(2)} = \dots$$

Nov 11, 2019

DEGENERATE PERTURBATION

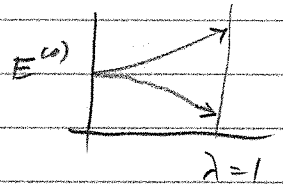
System with N states with same energy...

$$H^{(0)}|\psi_n^{(0)}\rangle = E^{(0)}|\psi_n^{(0)}\rangle \qquad n=1,\dots,N$$

But

$$\langle\psi_n^{(0)}|\psi_m^{(0)}\rangle = \delta_{mn}$$

We want lin. com of $|\psi_n^{(0)}\rangle$ where H' breaks degeneracy..



this is also a sum, but we're not gonna care...

Let $|\psi\rangle$ be $|\psi\rangle = \sum_i c_i|\psi_{n,i}^{(0)}\rangle + \lambda|\psi_n^{(1)}\rangle$

$$\Rightarrow H^{(0)}\sum_i c_i|\psi_{n,i}^{(0)}\rangle = \sum_i E_n^{(0)}c_i|\psi_{n,i}^{(0)}\rangle$$

Put into SE & Expand..

$$(H^{(0)}+\lambda H')|\psi\rangle = E|\psi\rangle$$. Like before $E = E_n^{(0)} + \lambda E_n^{(1)}$

Expand... $\cancel{H^{(0)}\sum_i c_i|\psi_{n,i}^{(0)}\rangle} + \lambda H'\sum_i c_i|\psi_{n,i}^{(0)}\rangle + H^{(0)}\lambda|\psi_n^{(1)}\rangle + \lambda^2 H'|\psi_n^{(1)}\rangle$

$$= \cancel{E_n^{(0)}\sum_i c_i|\psi_{n,i}^{(0)}\rangle} + E_n^{(0)}\lambda|\psi_n^{(1)}\rangle$$

$$+ E_n^{(1)}\lambda\sum_i c_i|\psi_{n,i}^{(0)}\rangle + \underbrace{\lambda^2 E_n^{(1)}|\psi_n^{(1)}\rangle}_{0,\,2^{nd}\text{ or}}$$

So to 1st order:

$$H^{(0)}|\psi_n^{(1)}\rangle + H'\sum_i c_i|\psi_{n,i}^{(0)}\rangle = E_n^{(0)}|\psi_n^{(1)}\rangle + \overset{\text{want this}}{E_n^{(1)}}\sum_i c_i|\psi_{n,i}^{(0)}\rangle$$

Multiply by $\langle\psi_{n,j}^{(0)}|$ → same energy but different states $j\neq i$

$$\langle \psi_{n,j}^{(0)} | H^{(0)} | \psi_n^{(1)} \rangle + \sum_i c_i \langle \psi_{nj}^{(0)} | H' | \psi_{n,i}^{(0)} \rangle$$

$$= E_n^{(0)} \langle \psi_{nj}^{(0)} | \psi_n^{(1)} \rangle + E_n^{(1)} \underbrace{\sum_i c_i \overset{\delta_{ij}}{\langle \psi_{nj}^{(0)} | \psi_{ni}^{(0)} \rangle}}_{c_j'}$$

$$\downarrow$$

$$\cancel{E_n^{(0)} \langle \psi_{nj}^{(0)} | \psi_n^{(1)} \rangle} + \sum_i c_i \langle \psi_{nj}^{(0)} | H' | \psi_{ni}^{(0)} \rangle$$

$$= \cancel{E_n^{(0)} \langle \psi_{nj}^{(0)} | \psi_n^{(1)} \rangle} + E_n^{(1)} c_j'$$

So

$$\boxed{\sum_i c_i \langle \psi_{nj}^{(0)} | H' | \psi_{ni}^{(0)} \rangle = E_n^{(1)} c_j'}$$

→ This is a matrix λ-value problem...

Look at 2-fold degeneracy... Two states with same energy...

$$H^{(0)} | \psi_{n1}^{(0)} \rangle = E_n^{(0)} | \psi_{n1}^{(0)} \rangle \;;\; H^{(0)} | \psi_{n2}^{(0)} \rangle = E_n^{(0)} | \psi_{n2}^{(0)} \rangle$$

But $\langle \psi_{n1}^{(0)} | \psi_{n2}^{(0)} \rangle = 0.$

Add perturbation H'... Build matrix elements...

$$H'_{11} = \langle \psi_{n1}^{(0)} | H' | \psi_{n1}^{(0)} \rangle$$

$$\boxed{H'_{ij} = \langle \psi_{ni}^{(0)} | H' | \psi_{nj}^{(0)} \rangle}$$

$$H'_{12} = \langle \psi_{n1}^{(0)} | H' | \psi_{n2}^{(0)} \rangle$$

$$H'_{21} = \langle \psi_{n2}^{(0)} | H' | \psi_{n1}^{(0)} \rangle$$

$$H'_{22} = \langle \psi_{n2}^{(0)} | H' | \psi_{n2}^{(0)} \rangle$$

For 2-fold, get 2 eqns

$$\left.\begin{aligned} c_1 H'_{11} + c_2 H'_{12} &= E_n^{(1)} c_1 \\ c_1 H'_{21} + c_2 H'_{22} &= E_n^{(1)} c_2 \end{aligned}\right\} \leftrightarrow \boxed{\begin{pmatrix} H'_{11} & H'_{12} \\ H'_{21} & H'_{22} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = E_n^{(1)} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}}$$

Ex $\{ 2D\ SHO + H' = \varepsilon m\omega^2 xy \}$

Full Hamiltonian: $H = \underbrace{\frac{p^2}{2m} + \frac{1}{2}m\omega^2(x^2+y^2)}_{H^{(0)}} + \underbrace{\varepsilon m\omega^2 xy}_{H'}$

Label states $|n_x\, n_y\rangle$. Energy $E_{n_x n_y} = (n_x + n_y + 1)\hbar\omega$

Ground state degenerate $|00\rangle$

1st excited state → 2-fold degeneracy $\langle 01|, \langle 10|$

$$\langle 01|10\rangle = 0.$$

Write H' in ladder ops ... $H' = \varepsilon m\omega^2 xy = \varepsilon m^2\, \hat{x} \cdot \hat{y}$

$$\rightarrow H' = \varepsilon m\omega^2 \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}_{+x} + \hat{a}_{-x}\right)\sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}_{+y} + \hat{a}_{-y}\right)$$

these are tensor products

$$= \varepsilon m\omega^2 \frac{\hbar}{2m\omega}\left(\hat{a}_{+x} + \hat{a}_{-x}\right)\left(\hat{a}_{+y} + \hat{a}_{-y}\right)$$

$$= \frac{\varepsilon\hbar\omega}{2}\left(\hat{a}_{+x}\hat{a}_{+y} + \hat{a}_{+x}\hat{a}_{-y} + \hat{a}_{-x}\hat{a}_{+y} + \hat{a}_{-x}\hat{a}_{-y}\right)$$

Look at

$$H'|10\rangle = \frac{\varepsilon\hbar\omega}{2}\left(\sqrt{2}\,|21\rangle + 0 + |01\rangle + 0\right)$$

$$H'|01\rangle = \frac{\varepsilon\hbar\omega}{2}\left(\sqrt{2}\,|12\rangle + |10\rangle + 0 + 0\right)$$

Find matrix elements...

$\langle 10|H'|10\rangle = 0$ $\qquad$ $\langle 10|H'|01\rangle = \frac{\varepsilon\hbar\omega}{2}$

$\langle 01|H'|10\rangle = \frac{\varepsilon\hbar\omega}{2}$ $\qquad$ $\langle 10|H'|10\rangle = 0$

So $H' = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \frac{\varepsilon\hbar\omega}{2} = \boxed{\frac{\varepsilon\hbar\omega}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = H'}$

So Eigenvalues & states...

$$E_+^{(1)} = \frac{\epsilon \hbar w}{2} \quad , \quad \frac{1}{\sqrt{2}}\left(|10\rangle + |01\rangle\right)$$

$$E_-^{(1)} = -\frac{\epsilon \hbar w}{2} \quad , \quad \frac{1}{\sqrt{2}}\left(|10\rangle - |01\rangle\right)$$

Total energies for these states...

$$\boxed{E = 2\hbar w \pm \epsilon \frac{\hbar w}{2}}$$

Nov 13, 2019 $\boxed{\text{Ex}}$ $H = V_0 \begin{pmatrix} 1-\epsilon & & \\ & 1 & \epsilon \\ & \epsilon & 2 \end{pmatrix}$ $\epsilon << 1$.

Unperturbed → $\epsilon = 0 \Rightarrow H^{(0)} = V_0 \begin{pmatrix} 1 & & \\ & 1 & \\ & & 2 \end{pmatrix}$

→ diagonal matrix → $\lambda_1 = V_0$, $\lambda_2 = V_0$, $\lambda_3 = 2V_0$.

Eigenstates: $|1\rangle = (1\ 0\ 0)^T$
$|2\rangle = (1\ 0\ 0)^T$
$|3\rangle = (0\ 0\ 1)^T$
} degenerate...

Full H: $\det(H - \lambda I) = 0 \Leftrightarrow \boxed{\lambda = V_0(1-\epsilon)}$

$$\lambda = \frac{V_0}{2}\left(3 \pm \sqrt{1+4\epsilon^2}\right)$$

Expand λ_2, λ_3 to get 1st order...

$$\sqrt{1+4\epsilon^2} \simeq 1 + 2\epsilon^2 + \dots \rightarrow \lambda_2 \simeq \frac{V_0}{2}\left(3 \pm (1+2\epsilon^2)\right)$$

So

$$\boxed{\begin{aligned} \lambda_2 &\simeq \frac{V_0}{2}\left[2 - 2\epsilon^2\right] = V_0(1-\epsilon^2) \\ \lambda_3 &\simeq \frac{V_0}{2}\left[4 + 2\epsilon^2\right] = V_0\left[2 + \epsilon^2\right] \end{aligned}}$$

no first order in ϵ.

(non-degenerate)

Perturbation theory $H' = \varepsilon V_0 \begin{pmatrix} -1 & & \\ & 0 & 1 \\ & 1 & 0 \end{pmatrix}$

- First order correction to $E_3^{(0)} = \lambda_3$...

$$E_3^{(1)} = \langle 3|H'|3\rangle = (0\ 0\ 1)\,\varepsilon V_0 \begin{pmatrix} -1 & & \\ & 0 & 1 \\ & 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0$$

$\Rightarrow$ no first order correction...

To first order, $E_3 = E_3^{(0)} + E_3^{(1)} = 2V_0$.

- Second order correction $E_3^{(2)}$

$$E_3^{(2)} = \sum_{m\neq 3} \frac{|\langle m|H'|3\rangle|^2}{E_3^{(0)} - E_m^{(0)}}$$

$$\langle 1|H'|3\rangle = \varepsilon V_0\,(1\ 0\ 0)\begin{pmatrix} -1 & & \\ & 0 & 1 \\ & 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0$$

$$\langle 2|H'|3\rangle = \varepsilon V_0\,(0\ 1\ 0)\begin{pmatrix} -1 & & \\ & 0 & 1 \\ & 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \varepsilon V_0$$

So $E_3^{(2)} = \dfrac{(\varepsilon V_0)^2}{E_3^{(0)} - E_2^{(0)}} = \dfrac{(\varepsilon V_0)^2}{V_0} = \boxed{\varepsilon^2 V_0}$

So to 2nd order $E_3^{(2)} = \underbrace{E_3^{(0)}}_{2} + \cancelto{0}{E_3^{(1)}} + E_3^{(2)} = \boxed{V_0(2+\varepsilon^2)}$

(degenerate)

Need to build 2x2 such that $H''_{11} = \langle 1|H'|2\rangle$
$H''_{12} = \langle 1|H'|2\rangle$
$H''_{21} = \langle 2|H'|1\rangle$
$H''_{22} = \langle 2|H'|2\rangle$

$H''_{11} = -\varepsilon V_0$ $\quad H''_{21} = 0$ $\quad \Rightarrow H'' = \varepsilon V_0 \begin{pmatrix} -1 & 0 \\ 0 & 0 \end{pmatrix}$
$H''_{12} = 0$ $\quad H''_{22} = 0$

Eigenvalues $E_1^{(1)} = -\varepsilon V_0 \Rightarrow \boxed{E_1 = E_1^{(0)} + E_1^{(1)} = V_0(1-\varepsilon)}$

$E_2^{(1)} = 0 \Rightarrow E_2 = E_2^{(0)} + E_2^{(1)} = V_0 \ldots$

Nov 14, 2019

HYDROGEN

Unperturbed $H^{(0)} = \frac{p^2}{2m} - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}$

Unperturbed energy: $E_n^{(0)} = \frac{-\alpha^2 m_e c^2}{2n^2}$ $\alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c} \sim \frac{1}{137}$,

Eigenstates $|n\, l\, m_l\, m_s\rangle = \psi_{nlm_l}(r,\theta,\varphi) \otimes \chi_I$

$E-|n|$

or L ang. mom

Z of angular mom

Z of spin...

Relativistic Correction $T = \sqrt{p^2c^2 + m_e^2c^4} - m_e c^2 \simeq \frac{p^2}{2m_e} - \frac{p^4}{8m_e^3c^2} + \ldots$

So, perturbation is $H' = \frac{-p^4}{8m_e^3c^2}$ (no spin involved...)

$$[H'_{ij}] = \langle n l_i m_{l_i} | H' | n l_j m_{l_j} \rangle$$

$$= \left\langle n l_i m_{l_i} \middle| \frac{-p^4}{8m_e^3c^2} \middle| n l_j m_{l_j} \right\rangle$$

Know

$$p^2 |n l m_l\rangle = 2m(E_n^{(0)} - V)|n l_j m_{l_j}\rangle$$

$$= \frac{-1}{8m_e^3c^2}\langle n l_i m_{l_i} | \vec{p}^2 \vec{p}^2 | n l_j m_{l_j}\rangle$$

$\boxed{\vec{p}^2 \text{ is Hermitian}}$

$$= \frac{-1}{8m_e^3c^2} \cdot \left[2m\,(E_n^{(0)} - V)\right]^2 \langle n l_i m_{l_i} | n l_j m_{l_j}\rangle$$

(VG)

$$= \frac{-(2m)^2}{8m_e^3c^2}\langle n l_i m_{l_i} | (E_n^{(0)} - V)^2 | n l_j m_{l_j}\rangle$$

radial operator...

$$= \frac{-(2m)^2}{8m^3c^2} \int \psi^{+}_{nl_i m_{l_i}} \, f(r) \, \psi_{nl_j m_{l_j}} \, d^3r$$

$$= \frac{-(2m)^2}{8m^3c^2} \int R_{nl_i}(r) \, f(r) \, R_{nl_j} \, dr \underbrace{\int Y_{l_i}^{m_{l_i}}(\theta,\varphi) \, Y_{l_j}^{m_{l_j}}(\theta,\varphi) \, d\Omega}$$

$$= \frac{-(2m)^2}{8m^3c^2} \int R_{nl_i} \, (E_n^{(0)}-V)^2 R_{nl_j} \, dr \cdot \delta_{l_i l_j} \delta_{m_{l_j} m_{l_i}}$$

$$= \frac{-(2m)^2}{8m^3c^2} \int R_{nl_i} \, (E_n^{(0)}-V)^2 R_{nl_j} \, dr \cdot \delta_{ij} \rightarrow \boxed{[H'] \text{ is diagonal}}$$

→ only nonzero entries are $\frac{-(2m)^2}{8m^3c^2} \int R_{nl} (E_n^{(0)}-V)^2 R_{nl} \, dr$.

$$\frac{-e^2}{4\pi\varepsilon_0} \frac{1}{r}$$

$$E_{rel}^{(1)} = \langle n \, l \, m_l | H' | n \, l \, m_l \rangle$$

$$= \frac{-4m^2}{8m^3c^2} \langle n \, l \, m_l | E_n^{(0)2} - 2E_n^{(0)} V + V^2 | n \, l \, m_l \rangle$$

$$= \frac{-4m^2}{8m^3c^2} (E_n^{(0)})^2 + \frac{8m^2 E_n^{(0)}}{8m^3c^2} \langle n l m_l | V | n l m_l \rangle - \frac{4m^2}{8m^3c^2} \langle n \, l \, m_l | V^2 | n l m_l \rangle$$

$$= \frac{-4m^2}{8m^3c^2} (E_n^{(0)})^2 + \frac{8m^2 E_n^{(0)}}{8m^3c^2} \cdot \frac{-e^2}{4\pi\varepsilon_0} \langle n l m_l | \frac{1}{r} | n l m_l \rangle - \frac{4m^2}{8m^3c^2} \cdot \left(\frac{-e^2}{4\pi\varepsilon_0}\right)^2 \langle n l m_l | 1/r^2 | n l m_l \rangle$$

$$\Rightarrow \boxed{E_{rel}^{(1)} = \frac{-1}{mc^2} (E_n^{(0)})^2 + \frac{E_n^{(0)}}{mc^2} \frac{-e^2}{4\pi\varepsilon_0} \langle 1/r \rangle + \frac{-1}{2mc^2} \left(\frac{-e^2}{4\pi\varepsilon_0}\right)^2 \left\langle \frac{1}{r^2} \right\rangle}$$

These expectation values are

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{n^2 a_0} = \frac{1}{n^2} \frac{me^2}{4\pi\varepsilon_0 \hbar^2}$$

$$\left\langle \frac{1}{r^2} \right\rangle = \frac{1}{(l+\frac{1}{2})\, n^3 a_0^2} \rightsquigarrow \text{splitting due to } l \ldots$$

Putting everything together...

$$E_{rel}^{(1)} = \frac{-1}{2mc^2}\left((E_n^{(0)})^2 + E_n^{(0)} \cdot \frac{e^2}{2\pi\varepsilon_0} \frac{me^2}{4\pi\varepsilon_0 \hbar^2} \cdot \frac{1}{n^2} + \frac{e^4}{16\pi^2\varepsilon_0^2} \cdot \frac{1}{(l+\frac{1}{2})n^3} \cdot \left(\frac{m_e e^2}{4\pi\varepsilon_0\hbar^2}\right)^2 \right)$$

<u>Recall</u> $\alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c}$, $E_n^{(0)} = \frac{-1}{2}\alpha^2 m_e c^2 \frac{1}{n^2}$

So,
$$E_{rel}^{(1)} = \frac{-1}{2mc^2}\left((E_n^{(0)})^2 - 4(E_n^{(0)})^2 + \frac{4n}{l+\frac{1}{2}}(E_n^{(0)})^2 \right)$$

$$\boxed{E_{rel}^{(1)} = \frac{-(E_n^{(0)})^2}{2mc^2}\left[\frac{4n}{l+\frac{1}{2}} - 3\right]} \rightsquigarrow \text{slightly lifted degeneracy with } l \ldots$$

↑ proportional to $\alpha^4 mc^2 \ldots$

Nov 15, 2019

$\boxed{\text{Spin-Orbit Coupling}}$ → another α^4 correction...

In electron frame, proton is orbiting + create B field → $H = -\vec{\mu}_e \cdot \vec{B}$ where

$$\vec{B} = \frac{\mu_0 I}{2r} \text{ where } I = \frac{e}{T} \rightarrow \text{period of orbit}$$

$$L_e = r m_e v = \frac{2\pi m e r^2}{T} \rightarrow \frac{1}{T} = \frac{L_e}{2\pi m_e r^2}$$

Put this into $\vec{B}$ eqn...

$$\rightarrow \boxed{\vec{B} = \frac{1}{4\pi\varepsilon_0} \frac{e}{m_e c^2 r^3} \vec{L}} \quad \text{since } c = \frac{1}{\sqrt{\mu_0 \varepsilon_0}}.$$

$\vec{\mu} = \gamma \vec{S}$. From EM, μ of ring of charge is $\boxed{\mu = \frac{q\pi r^2}{T}}$

Angular momentum of ring of charge is $S = \frac{2\pi m r^2}{T}$ $(mr^2 = I)$

$$\rightarrow \boxed{\vec{\mu}_e = \left(\frac{q}{2m}\right)\vec{S}} \rightsquigarrow \text{classical} \ldots$$

Because e^- is relativistic, $\boxed{\vec{\mu}_e = \frac{-e}{m_e}\vec{S}_e}$

and so ...

$$H' = -\vec{\mu}_e \cdot \vec{B} = \left(\frac{e^2}{4\pi\epsilon_0}\right)\left(\frac{1}{m_e^2 c^2 r^3}\right)\vec{S}\cdot\vec{L}$$

Because electron is accelerating ...

$$\boxed{H' = \left(\frac{e^2}{8\pi\epsilon_0}\right)\left(\frac{1}{m_e^2 c^2 r^3}\right)\vec{S}\cdot\vec{L}}$$

Expand dot product ...

$$\boxed{\begin{aligned}\vec{S}\cdot\vec{L} &= S_x L_x + S_y L_y + S_z L_z \qquad (\otimes) \\ &= \frac{1}{4}(S_+ + S_-)(L_+ + L_-) - \frac{1}{4}(S_+ - S_-)(L_+ - L_-) \\ &\qquad + S_z L_z\end{aligned}}$$

Defn

$$\boxed{\begin{aligned} S_+ |n l m_\ell m_s\rangle &= \alpha_+ |n l m_\ell m_s + 1\rangle \\ S_- |n l m_\ell m_s\rangle &= \alpha_- |n l m_\ell m_s - 1\rangle \\ L_+ |n l m_\ell m_s\rangle &= \beta_+ |n l m_\ell + 1 m_s\rangle \\ L_- |n l m_\ell m_s\rangle &= \beta_- |n l m_\ell - 1 m_s\rangle \end{aligned}}$$

Look at $\langle n l m_\ell m_s | \vec{S}\cdot\vec{L} | n l' m_\ell' m_s'\rangle$

$$= \langle n l m_\ell m_s | \tfrac{1}{2}(S_+ L_- + S_- L_+) + S_z L_z | n l' m_\ell' m_s'\rangle$$

$$= \frac{1}{2}\left\{\alpha_+\beta_- \langle n l m_\ell m_s | n l' m_\ell' - 1\ m_s' + 1\rangle + \alpha_-\beta_+ \langle n l m_\ell m_s | n l' m_\ell' + 1\ m_s' - 1\rangle\right\}$$

$$+ \hbar^2 m_\ell' m_s' \langle n l m_\ell m_s | n l' m_\ell' m_s'\rangle$$

$$= \frac{1}{2}\left\{\alpha_+\beta_- \delta_{\ell\ell'}\delta_{m_\ell m_\ell'-1}\delta_{m_s m_s'+1} + \alpha_-\beta_+ \delta_{\ell\ell'}\delta_{m_\ell m_\ell'+1}\delta_{m_s m_s'-1}\right\} + \hbar^2 m_\ell' m_s' \delta_{\ell\ell'}$$

Notice that because of the form of $\delta \Rightarrow H$ is not diagonal in this form.

Instead, we can use $\vec{J} = \vec{S} + \vec{L}$, then

$$\vec{J}^2 = \vec{L}^2 + \vec{S}^2 + 2\vec{S}\cdot\vec{L}, \text{ i.e. } \boxed{\vec{S}\cdot\vec{L} = \frac{1}{2}\left(\vec{J}^2 - \vec{L}^2 - \vec{S}^2\right)}$$

Remember that $\boxed{|l-s| \le j \le l+s \text{ and } m_j = m_l + m_s}$

↳ "good" quantum numbers are n, l, s, j, m_j.

If we do...

$$\langle n l s j m_j | \tfrac{1}{2}(\vec{J}^2 - \vec{L}^2 - \vec{S}^2) | n l' s j' m_j' \rangle$$

$$= \boxed{\frac{\hbar^2}{2}\left\{ j(j'+1) - l'(l'+1) - \frac{3}{4}\right\} \delta_{ll'}\delta_{jj'}\delta_{m_j m_j'}} \longrightarrow \text{diagonal}$$

So...

$$E^{(1)}_{S.O.} = \left\langle n l s j m_j \right| \frac{e^2}{8\pi\varepsilon_0}\cdot\frac{1}{m^2c^2r^3}\,\vec{S}\cdot\vec{L} \left| n l s j m_j \right\rangle$$

$$= \frac{e^2}{8\pi\varepsilon_0}\cdot\frac{1}{m^2c^2}\,\frac{\hbar^2}{2}\left\{ j(j+1) - l(l+1) - \frac{3}{4}\right\}\left\langle n l s j m_j \right| \frac{1}{r^3} \left| n l s j m_j \right\rangle$$

$$\boxed{E^{(1)}_{S.O.} = \frac{e^2}{8\pi\varepsilon_0}\cdot\frac{1}{m^2c^2}\cdot\frac{\hbar^2}{2}\left\{ j(j+1) - l(l+1) - \frac{3}{4}\right\}\left\langle \frac{1}{r^3}\right\rangle}$$

What is $\left\langle \frac{1}{r^3} \right\rangle$? $\rightsquigarrow \frac{1}{l(l+\frac{1}{2})(l+1)n^3a_0^3}$

So $$E^{(1)}_{S.O.} = \frac{e^2}{8\pi\varepsilon_0}\cdot\frac{1}{m^2c^2}\cdot\frac{\hbar^2}{2}\cdot\left\{ j(j+1) - l(l+1) - \frac{3}{4}\right\}\cdot\frac{1}{l(l+\frac{1}{2})(l+1)n^3a_0^3}$$

$$\Rightarrow \boxed{E^{(1)}_{S.O.} = \frac{e^2\hbar^2}{16\pi\varepsilon_0 m_e^2c^2}\;\frac{j(j+1) - l(l+1) - 3/4}{l(l+\frac{1}{2})(l+1)n^3a_0^3}} \rightsquigarrow \underline{0 \text{ when } l = 0.}$$

$$\boxed{H_Z' = -(\vec{\mu}_E + \vec{\mu}_S) \cdot \vec{B}_{ext}} = -\left(\cancel{\mu}\,\frac{-e}{2m_e}\vec{L} + \frac{-e}{m_e}\vec{S}\right) \cdot \vec{B}_{ext}$$

$$\boxed{H_Z' = \frac{e}{m_e}\left(\vec{L} + 2\vec{S}\right) \cdot \vec{B}_{ext}}$$

If $\vec{B}_{ext} \ll \vec{B}_{int}$ then H_Z' is a perturbation. (weak field)
If $\vec{B}_{ext} \gg \vec{B}_{int}$ then fine structure is the perturbation

Weak Field Zeeman Effect

$$H^{(0)} = H_{Bohr} + H_{fs}' \rightsquigarrow ~~[illegible]~~ \, (H_{so} + H_{rel})$$

and $H' = H_Z'$.

Because we have $\vec{L} + \vec{S}$, use $|n\, l\, j\, m_j\rangle$ as states.
Let $\vec{B}_{ext} = B_{ext} \cdot \hat{k}$, then

Energy correction: $E_Z^{(1)} = \langle n\, l\, j\, m_j | H_Z' | n\, l\, j\, m_j \rangle$

$$= \frac{e}{2m} B_{ext}\, \hat{k} \cdot \langle n l j m_j | \vec{L} + 2\vec{S} | n l j m_j \rangle$$

$$= \frac{e}{2m} B_{ext}\, \hat{k} \cdot \langle n l j m_j | \vec{J} + \vec{S} | n l j m_j \rangle$$

$\vec{J}$ is conserved, $\vec{L}$ & $\vec{S}$ not conserved separately.
Time averaged - value of $\vec{S}$ (projection along $\vec{J}$)

$$\boxed{\vec{S}_{ave} = \frac{(\vec{S} \cdot \vec{J})}{J^2}\vec{J}}$$

Write $\vec{L} = \vec{J} - \vec{S}$ and square, $\vec{L}^2 = \vec{J}^2 + \vec{S}^2 - 2\vec{S} \cdot \vec{J}$

$$\Rightarrow \vec{S} \cdot \vec{J} = \frac{1}{2}(J^2 + S^2 - L^2)$$

So, $\langle \vec{L} + 2\vec{S} \rangle = \langle \vec{J} + \vec{S} \rangle \sim \left\langle \vec{J} + \frac{(\vec{S} \cdot \vec{J})}{J^2} \cdot \vec{J} \right\rangle = \left\langle \left(1 + \frac{\vec{S} \cdot \vec{J}}{J^2}\right) \vec{J} \right\rangle$

Write this in terms of $E_n^{(0)}$...

$$\boxed{E^{(1)}_{s.o.} = \frac{(E_n^{(0)})^2}{m_e c^2}\,\frac{n(j(j+1) - l(l+1) - 3/4)}{l(l+1/2)(l+1)}} \rightarrow \sim \alpha^4$$

→ Full fine structure correction, is the sum of this & relativistic...

$$\boxed{E^{(1)}_{fs} = E^{(1)}_{rel} + E^{(1)}_{s.o.} = \frac{(E_n^{(0)})^2}{2 m_e c^2}\left(3 - \frac{4n}{j+1/2}\right)}$$

Combine this with unperturbed energy... (up to $O(\alpha^4)$)

$$E_{nj} = -\frac{E_1^{(0)}}{n^2} + \frac{(E_n^{(0)})^2}{2 m_e c^2}\left(3 - \frac{4n}{j+1/2}\right)$$

And since $E_n^{(0)} = \frac{-1}{2}\alpha^2 m_e c^2 / n^2$ ...

$$\boxed{E_{nj} = \frac{-\alpha^2 m_e c^2}{2n^2}\left(1 + \frac{\alpha^2}{n^2}\left\{\frac{n}{j+1/2} - \frac{3}{4}\right\}\right)} \rightarrow \text{broken degeneracy in } l \ldots$$

→ new degeneracy in j.

Zeeman - Lamb shift → lift degeneracy in j...

Nov 22, 2019

ZEEMAN EFFECT

$j = l \pm \frac{1}{2}$ ⇒ can get same j's for different l's.

$j = \frac{1}{2}$ with $l = 0$ (s) & $l = 1$ (p)

→ split between levels with same j but different l is called the LAMB SHIFT ($O(\alpha^5 m_e c^2)$)

→ measure by putting atom in $\vec{B}$ field...

For single e^- atom like H... Hamiltonian is...

$$= \left\langle \left(1 + \frac{1}{2} \frac{(J^2 + S^2 - L^2)}{J^2} \right) \vec{J} \right\rangle$$

$$= \boxed{\underbrace{\left\{ 1 + \frac{j(j+1) + s(s+1) - \ell(\ell+1)}{2j(j+1)} \right\}}_{\text{Landé } g_J\text{-factor}} \langle \vec{J} \rangle}$$

$$\boxed{\sim 2 \text{ for } H}$$

And so... $E_z^{(1)} \sim \frac{e}{2m} B_{ext} \cdot \hat{k} \cdot \langle \vec{J} + 2\vec{S} \rangle$ $\qquad \hat{k} \cdot \langle \vec{J} \rangle = \langle J_z \rangle$

$= m_j \hbar$

$$= \frac{e}{2m_e} B_{ext} (g_J) \, m_j \hbar$$

$$\boxed{E_z^{(1)} = \mu_B \, g_j \, B_{ext} \, m_j \quad , \; \mu_B = \frac{e\hbar}{2m_e}}$$ Bohr magneton

Energy split based on m_j : For $n = 1$, $\ell = 0$, $j = \frac{1}{2}$, $m_j = \pm\frac{1}{2}$

$g_j = 2$ for H

With these...
(weak field)
$$\boxed{E_1 = \underset{\uparrow \atop fs}{E_1^{(0)} \left(1 + \frac{\alpha^2}{4} \right)} \pm \underset{\uparrow \atop \text{Zeeman}}{\mu_B B_{ext}}}$$

#

When $B_{ext} \gg B_{int}$..., then $\begin{cases} H^{(0)} = H_{Bohr} + H_Z' \\ \text{and} \\ H' = H_{fs}' \end{cases}$

again assume that

$\vec{B}_{ext} = B_{ext} \hat{k}$, then

ℓ, s, m_ℓ
m_s are
good states... $\rightsquigarrow$ $\boxed{H_Z' = \frac{e}{2m} B_{ext} (L_z + 2S_z)}$ $\rightarrow$ want to use $| n \, \ell \, m_\ell \, m_s \rangle$ since we want m_ℓ, m_s...

$\rightarrow$ Unperturbed energies $\Rightarrow$ $\boxed{E^{(0)}_{n \ell m_\ell m_s} = \frac{E_1^{(0)}}{n^2} + \mu_B B_{ext} (m_\ell + 2m_s)}$

f-s correction is

$$\boxed{H'_{fs} = \frac{-p^4}{8m_e^3c^2} + \left(\frac{e^2}{8\pi\epsilon_0}\right)\left(\frac{1}{m_e^2c^2r^3}\right)\vec{S}\cdot\vec{L}}$$

First part is what we found before...

$$\boxed{E^{(1)}_{rel} = \frac{-(E_n^{(0)})^2}{2m_ec^2}\left(\frac{4n}{l+1/2} - 3\right)}$$

For the 2nd part need to look at $\vec{S}\cdot\vec{L}$...

$$\begin{aligned}\langle \vec{S}\cdot\vec{L}\rangle &= \langle S_xL_x\rangle + \langle S_yL_y\rangle + \langle S_zL_z\rangle \\ &= \langle S_x\rangle\langle L_x\rangle + \langle S_y\rangle\langle L_y\rangle + \langle S_z\rangle\langle L_z\rangle\end{aligned}$$

If we're in S_z, L_z eigenstates ⇒ $\langle S_{x,y}\rangle = \langle L_{x,y}\rangle = 0$

$$\Rightarrow \boxed{\langle \vec{S}\cdot\vec{L}\rangle = \langle S_z\rangle\langle L_z\rangle = \hbar^2 m_l m_s.}$$

We also know... $\left\langle\frac{1}{r^3}\right\rangle = \frac{1}{l(l+\frac{1}{2})(l+1)a_0^3n^3}$

Combine to find

$$\boxed{E^{(1)}_{fs} = \frac{E_1^{(0)}}{n^3}\alpha^2\left(\frac{3}{4n} - \underbrace{\frac{l(l+1)-m_lm_s}{l(l+1)(l+1/2)}}_{=1 \text{ when } l=0}\right)}$$

And so... combine to find E in strong field (1)...

$$\boxed{E_n^{(1)} = E_n^{(0)} + \mu_B B_{ext}(m_l + 2m_s) + \frac{E_1^{(0)}}{n^3}\alpha^2\left(\frac{3}{4n} - \frac{l(l+1)-m_lm_s}{l(l+1)(l+1/2)}\right)}$$

What about $H_{fs} \sim H_{Zeeman}$? ⇒ intermediate field...

$\boxed{\text{Intermediate field} \rightarrow H_{fs} \sim H_{Zeeman} \Rightarrow \text{Both are perturbations..}}$

$$H'_Z \simeq H'_{fs} \Rightarrow \boxed{\begin{aligned} H^{(0)} &= H_{Bohr} \\ H' &= H'_Z + H'_{fs} \end{aligned}}$$

☒ Focus on $n=2$ states... F.S. wants $|n\, j\, m_j\, m_s\rangle$ } not
Zeeman wants $|n\, l\, m_l\, m_s\rangle$ } compatible ...

But we can mix $|n\, l\, m_l\, m_s\rangle$ with $|n\, j\, m_j\, m_s\rangle$ & vice versa...
For $n=2$, 8 states...

$$|n\ l\ m_j\ m_s\rangle \qquad \boxed{n=2} \qquad |n\ l\ m_l\ m_s\rangle$$

$$\overset{\shortparallel}{|j\ m_j\rangle} \qquad\qquad \overset{\shortparallel}{|l\ s\ m_l\ m_s\rangle}$$

$l=0$

$$|1\rangle = |\tfrac{1}{2}\ \tfrac{1}{2}\rangle = |0\ 1/2\ 0\ 1/2\rangle$$

$$|2\rangle = |\tfrac{1}{2}\ \tfrac{-1}{2}\rangle = |0\ 1/2\ 0\ -1/2\rangle$$

$l=1$

$$|3\rangle = |3/2\ 3/2\rangle = |1\ 1/2\ 1\ 1/2\rangle$$

$$|4\rangle = |3/2\ -3/2\rangle = |1\ 1/2\ -1\ -1/2\rangle$$

$$|5\rangle = |3/2\ +1/2\rangle = \sqrt{2/3}\,|1\ 1/2\ 0\ 1/2\rangle + \sqrt{1/3}\,|1\ 1/2\ 1\ -1/2\rangle$$

$$|6\rangle = |1/2\ +1/2\rangle = -\sqrt{1/3}\,|1\ 1/2\ 0\ 1/2\rangle + \sqrt{\tfrac{2}{3}}\,|1\ 1/2\ 1\ -1/2\rangle$$

$$|7\rangle = |3/2\ -1/2\rangle = \sqrt{1/3}\,|1\ 1/2\ -1\ 1/2\rangle + \sqrt{2/3}\,|1\ 1/2\ 0\ 1/2\rangle$$

$$|8\rangle = |\tfrac{1}{2}\ -\tfrac{1}{2}\rangle = -\sqrt{\tfrac{2}{3}}\,|1\ 1/2\ -1\ \tfrac{1}{2}\rangle + \sqrt{\tfrac{1}{3}}\,|1\ \tfrac{1}{2}\ 0\ -\tfrac{1}{2}\rangle$$

ov 21, 2014

→ now, need to find $\langle f|H'|g\rangle$ $f, g = 1, 2, \ldots, 8$ → 8×8 matrix
~~because~~ but not gonna be diagonal ⇒ need to look at matrix.

Define $\boxed{\gamma = \left(\frac{\alpha}{8}\right)^2 E_1^{(0)}}$ and $\boxed{\beta = \mu_B B_{ext}}$

↑ fs ↑ Zeeman

$$-H' = \left(\begin{array}{cccc|cc|cc}
5\gamma-\beta & & & & & & & \\
 & 5\gamma+\beta & & & & & & \\
 & & \gamma-2\beta & & & & & \\
 & & & \gamma+2\beta & & & & \\
\hline
 & & & & \gamma-\tfrac{2}{3}\beta & \sqrt{\tfrac{2}{3}}\beta & & \\
 & & & & \sqrt{\tfrac{2}{3}}\beta & 5\gamma-\tfrac{1}{3}\beta & & \\
\cline{5-8}
 & & & & & & \gamma+\tfrac{2}{3}\beta & \sqrt{2}/_3\,\beta \\
 & & & & & & \sqrt{2}/_3\,\beta & 5\gamma+\tfrac{1}{3}\beta
\end{array}\right)$$

↑ direct sum of operators ... Easy to find eigenvalues...

8 energy corrections

$$\left\{\begin{aligned}
\varepsilon_1 &= E_2^{(0)} - 5\gamma + \beta \\
\varepsilon_2 &= E_2^{(0)} - 5\gamma - \beta \\
\varepsilon_3 &= E_2^{(0)} - \gamma + 2\beta \\
\varepsilon_4 &= E_2^{(0)} - \gamma - 2\beta \\
\varepsilon_5 &= E_2^{(0)} - 3\gamma + \beta/2 + \left(4\gamma^2 + \tfrac{2}{3}\beta + \beta^2/4\right)^{1/2} \\
\varepsilon_6 &= E_2^{(0)} - 3\gamma + \beta/2 - \left(4\gamma^2 + \tfrac{2}{3}\beta + \beta^2/4\right)^{1/2} \\
\varepsilon_7 &= E_2^{(0)} - 3\gamma - \beta/2 + \left(4\gamma^2 - \tfrac{2}{3}\beta + \beta^2/4\right)^{1/2} \\
\varepsilon_8 &= E_2^{(0)} - 3\gamma - \beta/2 - \left(4\gamma^2 - \tfrac{2}{3}\beta + \beta^2/4\right)^{1/2}
\end{aligned}\right.$$

→ broke all degeneracies...

The LAMB SHIFT

unperturbed $n = 2$ states all have $E_2^{(0)}$

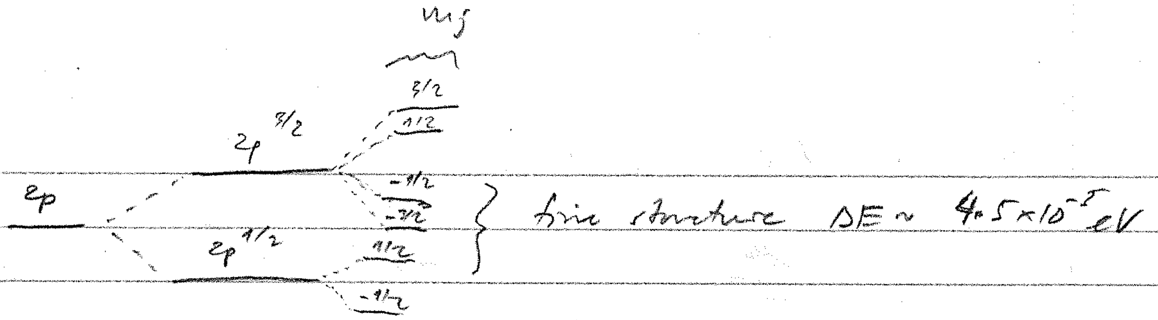
s states $(l = 0)$

p states $(l = 1)$

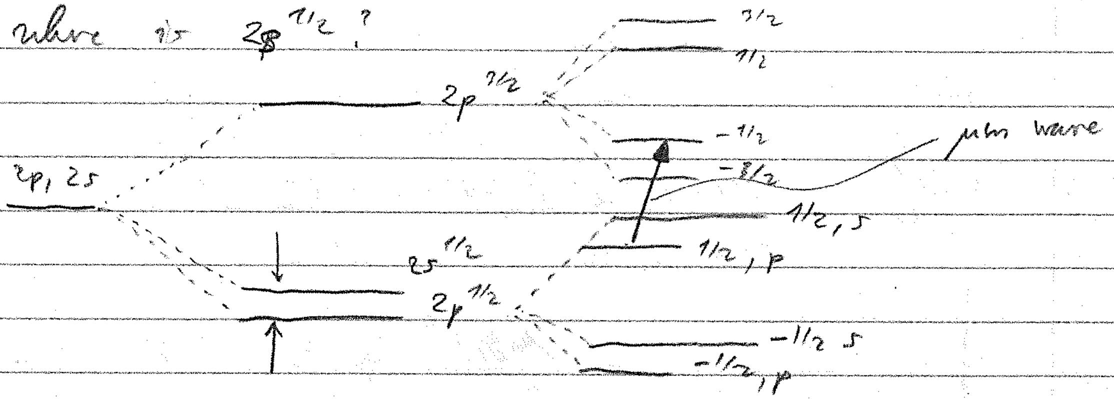
- Fine structure splits $2p^{1/2}$ from $2p^{3/2}$, but $2s^{1/2}$, $2p^{1/2}$ still the same.

$n = 2,\ l = 1$ $\qquad$ $n = 2,\ l = 1$ $\qquad$ (same j, n)

$j = 1/2$ $\qquad$ $j = 3/2$



where is $2s^{1/2}$?



Transition from $2p^{1/2} \to 2p^{3/2}$ by excitations to microwave
$2p^{3/2}$ can transition to $2s^{1/2}$

ΔE between $2p^{1/2}$ & $2s^{1/2}$ ≃ 4.372×10^{-6} eV

HYPERFINE STRUCTURE

↳ takes the proton into account
↳ spin of proton & spin of electron...

→ This is a spin-spin interaction between proton & electron.

Magnetic dipole moment of proton sets up magnetic field
(different from that caused by its motion)

We know
$$\boxed{\begin{aligned}\vec{\mu}_e &= \frac{-e}{m_e}\vec{S}_e \\ \Rightarrow \vec{\mu}_p &= \frac{g_p e}{2m_p}\vec{S}_p\end{aligned}}$$
(spin ... not orbital ang. mom.)

$$-\frac{g_e e}{2m_e}\vec{S}_e = \frac{-e}{m_e}\vec{S}_e, \quad g_e \sim 2.00\ldots$$

strength factor is not 2, rather = 5.59

$$\boxed{\text{Since } m_p \ll m_e \Rightarrow \vec{\mu}_p \ll \vec{\mu}_e}$$

Magnetic field of a dipole is

$$\boxed{\vec{B}_{\mu_p (p)} = \frac{\mu_0}{4\pi r^3}\left[3(\vec{\mu}_p\cdot\vec{r})\hat{r} - \vec{\mu}_p\right] + \frac{2\mu_0}{3}\vec{\mu}_p\,\delta^{(3)}(\vec{r})}$$

Interaction is $\vec{\mu}_e\cdot\vec{B}$

$$\boxed{\begin{aligned} H'_{hf} &= \frac{\mu_0 g_p e^2}{8\pi m_p m_e}\left\{\frac{3(\vec{S}_p\cdot\hat{r})(\vec{S}_e\cdot\hat{r}) - \vec{S}_p\cdot\vec{S}_E}{r^3}\right\} && (A) \\ &\quad + \frac{\mu_0 g_p e^2}{3 m_p m_e}\vec{S}_p\cdot\vec{S}_e\,\delta^{(3)}(\vec{r}) && (B)\end{aligned}}$$

Look at ground state, $l=0$, $\left\langle\frac{1}{r^3}\right\rangle = \frac{1}{l(l+1)(l+1/2)a_0^3 n^3} - 1$ for $l=0$.

Problem 7.31 shows that expectation value of $(A)=0$ $\forall\, l=0$. With this, left with

$$\boxed{E^{(1)}_{hf} = \frac{\mu_0 g_p e^2}{3 m_e m_p}\langle\vec{S}_p\cdot\vec{S}_e\rangle \underbrace{|\psi_{100}(0)|^2}_{} \longrightarrow \langle\delta^{(3)}(\vec{r})\rangle}$$

know $|\psi_{100}(0)|^2 = \frac{1}{\pi a_0^3}$ ... so,

$$\boxed{E^{(1)}_{hf} = \frac{\mu_0 g_p e^2}{3 m_e m_p \pi a_0^3}\langle\vec{S}_e\cdot\vec{S}_p\rangle}$$

Use triplet + singlet states ... since $\vec{S} = \vec{S}_e + \vec{S}_p$

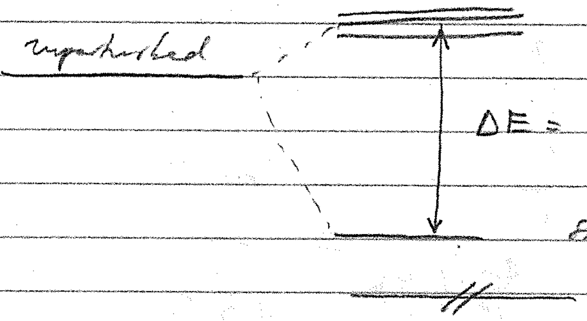
so $\left(\vec{S}_e\cdot\vec{S}_p = \frac{1}{2}\left(\vec{S}^2 - \vec{S}_e^2 - \vec{S}_p^2\right)\right) \rightarrow$ both e, p have $s=\frac{1}{2}$

$\Rightarrow \vec{S}_e^2 = \vec{S}_p^2 = \frac{1}{2}\left(\frac{1}{2}+1\right)\hbar^2 = \frac{3\hbar^2}{4}$

Triplet ... $s=1 \Rightarrow S^2 = 1(1+1)\hbar^2 = \boxed{2\hbar^2}$ Singlet $s=0 \Rightarrow \boxed{S^2=0}$

So, can write...

$$\boxed{E_{hf}^{(1)} = \frac{4 g_p \hbar^4}{3 m_p m_e^2 c^2 a_0^4}\begin{cases} 1/4 & \text{triplet} \\ -3/4 & \text{singlet}\end{cases}}$$



$\Delta E = 5.88\times 10^{-6}\,\text{eV}$, $\nu = \frac{\Delta E}{h} = 1420\,\text{MHz}$ $\boxed{\lambda = 21\,\text{cm}}$

a lot in universe...

Nov 21, 2019

$\boxed{\text{Ex}}$ Particle in 2D ∞ well...

$$V = \begin{cases} 0 & 0<x<L,\ 0<y<L \\ \infty & \text{else...}\end{cases}$$

$$\boxed{|n_x n_y\rangle = \left(\sqrt{\frac{2}{L}}\right)^2 \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right) \Rightarrow E_{xy}^{(0)} = \frac{\pi^2\hbar^2}{2mL^2}(n_x^2+n_y^2)}$$

So

$$E_{11}^{(0)} = \frac{\pi^2\hbar^2}{mL^2}$$

First excited states: $E_{12}^{(0)} = E_{21}^{(0)}$ → doubly degenerate

$$\begin{cases} |12\rangle = \frac{2}{L}\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi y}{L}\right) \\ |21\rangle = \frac{2}{L}\sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right)\end{cases} \qquad \boxed{E_{12}^{(0)} = E_{21}^{(0)} = \frac{5\hbar^2\pi^2}{2mL^2}}$$

Add perturbation

$$H' = \begin{cases} \lambda & 0\le x\le L/2,\ 0\le y\le \frac{L}{2} \\ 0 & \text{else...}\end{cases}$$

Ground state → non degenerate pert theory → $\boxed{E_{11}^{(1)} = \langle 11|H'|11\rangle}$

$$E_{11}^{(1)} = \langle 11|H'|11\rangle = \frac{4\lambda}{L^2}\int_0^{L/2}\int_0^{L/2} \sin^2\left(\frac{\pi x}{L}\right)\sin^2\left(\frac{\pi y}{L}\right) dx\,dy$$

$$= \frac{4\lambda}{L^2}\left(\int_0^{L/2} \sin^2\frac{\pi x}{2}\right)^2 = \frac{1}{4}\frac{4\lambda}{L^2}\left[\int_0^{L/2} 1-\cos\frac{2\pi x}{L}\,dx\right]^2$$

$$= \frac{2\lambda}{L^2}\left(\frac{L}{2} - \frac{L}{2\pi}\cdot\sin\left(\frac{2\pi x}{L}\right)\Big|_0^{L/2}\right)^2$$

$$= \frac{2\lambda}{L^2}\left(\frac{L}{2} - \frac{L}{2\pi}\underset{0}{\left(\cancel{\sin(\pi)}\right)}\right)^2$$

$$= \frac{2\lambda}{L^2}\left(\frac{L}{2}\right)^2 = \boxed{\frac{\lambda}{4}}$$

So $\boxed{E_{11}^{(1)} = \frac{\lambda}{4}}$

First excited states... look at $\langle 12|H'|12\rangle$, $\langle 12|H'|21\rangle$
$\langle 21|H'|12\rangle$, $\langle 21|H'|12\rangle$

$$\langle 12|H'|12\rangle = \frac{4\lambda}{L^2}\left\{\int_0^{L/2} \sin^2\left(\frac{\pi x}{L}\right)\sin^2\left(\frac{2\pi y}{L}\right)\right\} dx\,dy$$

$$= \frac{4\lambda}{L^2}\cdot\left(\frac{L}{4}\right)\int_0^{L/2}\sin^2\left(\frac{2\pi y}{L}\right) dy$$

$$= \frac{4\lambda}{L^2}\cdot\frac{L}{4}\cdot\frac{L}{4} = \boxed{\frac{\lambda}{4}}$$

Similarly, by symmetry, $\langle 21|H'|12\rangle = \boxed{\lambda/4}$

Okay... $\langle 12|H'|21\rangle = \frac{4\lambda}{L^2}\int_0^{L/2}\int_0^{L/2} \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi y}{L}\right)\sin\left(\frac{2\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right) dy\,dx = 0$

$\quad\quad ||$

$\langle 21|H'|12\rangle$

$$= \frac{4\lambda}{L^2}\left\{\int_0^{L/2}\sin\frac{\pi x}{L}\sin\frac{2\pi x}{L}\,dx\right\}^2$$

$$= \frac{4\lambda}{L^2}\left\{\int_0^{L/2} 2\sin^2\frac{\pi x}{L}\cdot\cos\frac{\pi x}{L}\,dx\right\}^2$$

$$= \frac{4\lambda}{L^2}\cdot 4\left(\int_0^{L/2}\sin^2\frac{\pi x}{L}\cos\frac{\pi x}{L}\,dx\right)^2$$

$$\langle 12|H'|21\rangle = \langle 21|H'|12\rangle = \frac{16\lambda}{L^2}\left\{\int_0^1 \left(\frac{\pi}{L}\right)^{-1} u^2\,du\right\}^2 \qquad u = \sin\frac{\pi x}{L}$$

$$= \left(\frac{L}{\pi}\right)\frac{16\lambda}{L^2}\left(\int_0^1 u^2\,du\right)^2 \qquad du = \left(\cos\frac{\pi x}{L}\right)\frac{\pi}{L}dx$$

$$= \frac{16\lambda}{\pi^2}\cdot\left(\frac{1}{3}\right)^2 = \boxed{\frac{16\lambda}{9\pi^2}}$$

So

$$\boxed{H'_{ij} = \lambda\begin{pmatrix} 1/4 & 16/9\pi^2 \\ 16/9\pi^2 & 1/4 \end{pmatrix}}$$

Now, diagonalize...

$$\left(\lambda/4 - \xi\right)^2 - \left(\frac{16\lambda}{9\pi^2}\right)^2 = 0 \Leftrightarrow \frac{\lambda^2}{16} - \frac{\xi\lambda}{2} + \xi^2 - \left(\frac{16\lambda}{9\pi^2}\right)^2 = 0$$

$$\Leftrightarrow \quad \xi^2 - \frac{\lambda}{2}\xi + \frac{\lambda^2}{16} - \left(\frac{16\lambda^2}{9\pi^2}\right)^2 = 0$$

$$\Leftrightarrow \quad \xi = \frac{\lambda/2 \pm \sqrt{\lambda^2/4 - 4\left(\lambda^2/16 - \left(16\lambda/9\pi^2\right)^2\right)}}{2}$$

$$\boxed{\xi_\pm = \frac{\lambda}{4} \pm \left(\frac{16\lambda}{9\pi^2}\right)}$$

need to find eigenvectors.. to get the correct basis states...

$$\begin{pmatrix} \lambda/4 & 16\lambda/9\pi^2 \\ 16\lambda/9\pi^2 & \lambda/4 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \left(\lambda/4 \pm \frac{16\lambda}{9\pi^2}\right)\begin{pmatrix} a \\ b \end{pmatrix}$$

$$\begin{pmatrix} \frac{a}{4} + \frac{16}{9\pi^2}b \\ \frac{16}{9\pi^2}a + a/4 \end{pmatrix} = \begin{pmatrix} a/4 \pm 16/9\pi^2\, a \\ b/4 \pm 16/9\pi^2\, b \end{pmatrix} \quad \vec{x}_+ = \begin{pmatrix} 1 \\ 1 \end{pmatrix}\frac{1}{\sqrt{2}} \quad \& \quad \vec{x}_- = \begin{pmatrix} 1 \\ -1 \end{pmatrix}\frac{1}{\sqrt{2}}$$

$$\Rightarrow \quad \vec{x}_+ = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}; \quad \vec{x}_- = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

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Call ... $|+\rangle = \frac{1}{\sqrt{2}}\left(|12\rangle + |21\rangle\right)$ & $|12\rangle = \begin{pmatrix}1\\0\end{pmatrix} \rightarrow$ org basis

$$|-\rangle = \frac{1}{\sqrt{2}}\left(|12\rangle - |21\rangle\right)$$

So
$$\boxed{\begin{aligned} E_+ &= \frac{5\pi^2\hbar^2}{2mL^2} + \frac{\lambda}{4} + \frac{16\lambda}{9\pi^2} \\ E_- &= \frac{5\pi^2\hbar^2}{2mL^2} + \frac{\lambda}{4} - \frac{16\lambda}{9\pi^2} \end{aligned}}$$

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Nov 22 2019

$\boxed{\text{Ex}}$ 3D SHO + $\frac{1}{2}k\,\delta xy$, $\omega = \sqrt{k/m}$

$$\boxed{\begin{aligned} H^{(0)} &= \frac{p^2}{2m} + \frac{1}{2}m\omega^2(x^2+y^2+z^2) \\ H' &= \frac{1}{2}m\omega^2 xy \end{aligned}}$$

Label states $|n_x n_y n_z\rangle$, $E^{(0)}_{n_x n_y n_z} = (n_x + n_y + n_z + \frac{3}{2})\hbar$

$x = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}_{+x} + \hat{a}_{-x}\right)$; $y = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}_{+y} + \hat{a}_{-y}\right)$

Gnd state ... $|000\rangle$

$$xy = \frac{\hbar}{2m\omega}\left(\hat{a}_{+x}\hat{a}_{+y} + \hat{a}_{-x}\hat{a}_{-y} + \hat{a}_{+x}\hat{a}_{+y} + \hat{a}_{-x}\hat{a}_{-y}\right)$$

$$\begin{cases} \hat{a}_{+x}\hat{a}_{+y}|000\rangle = 1.1.|110\rangle \\ \hat{a}_{+x}\hat{a}_{-y}|000\rangle = 0 \\ \hat{a}_{-x}\hat{a}_{+y}|000\rangle = 0 \\ \hat{a}_{-x}\hat{a}_{-y}|000\rangle = 0 \end{cases}$$

constant

$$E^{(1)}_{000} = \langle 000|H'|000\rangle = \langle 000|\cdots|110\rangle = 0$$

$\rightarrow$ no first order correction.

non-degenerate ... $E^{(2)}_{000} = \sum\limits_{\text{not}} \frac{|\langle n_x n_y n_z|H'|000\rangle|^2}{E^{(0)} - E^{(0)}}$

So $E^{(2)}_{000} = ?$ only $\langle 110|$ term survives...

$$E^{(0)}_{110} = \frac{7}{2}\hbar\omega$$

$$E^{(0)}_{000} - E^{(0)}_{110} = \left(\frac{3}{2}-\frac{7}{2}\right)\hbar\omega = -2\hbar\omega \ldots$$

So
$$E^{(2)}_{000} = \sum \frac{|\langle n_x n_y n_z|H'|000\rangle|^2}{E^{(0)}_{000}-E^{(0)}_{110}}$$

$$= \frac{1}{-2\hbar\omega}\cdot\left(\frac{\hbar}{2m\omega}\right)^2\cdot\left(\frac{1}{2}k\right)^2 \longrightarrow \frac{1}{2}(m\omega^2)^2$$

$$= \boxed{\frac{-1}{32}\hbar\omega}$$

First excited state $|001\rangle, |100\rangle, |010\rangle$.

$$E^{(0)}_{100} = E^{(0)}_{010} = E^{(0)}_{001} = \frac{5}{2}\hbar\omega \rightarrow \text{degenerate}\ldots$$

Are these eigenstates of H'?

$xy|100\rangle = ?$

$\hat{a}_{+x}\hat{a}_{+y}|100\rangle = \sqrt{2}|210\rangle$; $\sqrt{2}|120\rangle$

$\hat{a}_{-x}\hat{a}_{+y}|100\rangle = |010\rangle$; 0

$\hat{a}_{+x}\hat{a}_{-y}|100\rangle = 0$; $|100\rangle$

$\hat{a}_{-x}\hat{a}_{-y}|100\rangle = 0$; 0

$\hat{a}_{+x}\hat{a}_{+y}|001\rangle = |111\rangle$

$\hat{a}_{-x}\hat{a}_{+y}|001\rangle = 0$

$\hat{a}_{-x}\hat{a}_{-y}|001\rangle = 0$

$\hat{a}_{+x}\hat{a}_{-y}|001\rangle = 0$

What is matrix? → only nonzero terms are $\langle 010|H'|100\rangle$
$\langle 100|H'|010\rangle$

$$\boxed{H' = \frac{1}{4}\hbar\omega\begin{pmatrix}0&1&0\\1&0&0\\0&0&0\end{pmatrix}}$$

Eigenvalues: $(\pm 1, 0)\,\frac{1}{4}\hbar\omega = \boxed{\pm\frac{1}{4}\hbar\omega,\ 0}$

Eigenstates:

$$\hookrightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Rightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \text{ or } \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

First excited state

$$\boxed{\begin{aligned} |1\rangle &= \frac{1}{\sqrt{2}}\left\{ |100\rangle + |010\rangle \right\} \\ E_1^{(1)} &= \frac{5}{2}\hbar\omega + \frac{1}{4}\hbar\omega \\ |2\rangle &= \frac{1}{\sqrt{2}}\left\{ |100\rangle - |010\rangle \right\} \\ E_2 &= \frac{5}{2}\hbar\omega - \frac{1}{4}\hbar\omega \\ |3\rangle &= |001\rangle \\ E_3 &= \frac{5}{2}\hbar\omega \end{aligned}}$$

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Nov 25, 2019

$\boxed{\text{NEXT: TIME-DEPENDENT PERTURBATION THEORY}}$

Time independent System: $H^{(0)} \rightarrow H^{(0)}|\Psi_n^{(0)}\rangle = E_n^{(0)}|\Psi_n^{(0)}\rangle$

Time dependent potential $V(t)$ $\hookrightarrow \langle \Psi_n^{(0)} | \Psi_m^{(0)} \rangle = \delta_{mn}$

$$\boxed{H = H^{(0)} + V(t)}$$

General unperturbed state

$$\boxed{|\Psi^{(0)}\rangle = \sum_n c_n |\Psi_n\rangle e^{-iE_n^{(0)}t/\hbar}}$$ where c_n are time-indep.

Want solutions to time-dep SE: $\boxed{i\hbar\partial_t|\Psi\rangle = (H^{(0)} + V(t))|\Psi\rangle}$

Let $$\boxed{|\Psi\rangle = \sum_n c_n(t)\,|\psi_n^{(0)}\rangle e^{-iE_n^{(0)}t/\hbar}}$$

Want to find $c_n(t)$... When $V \to 0$, $c_n(t) \to c_n$, indep of tim

Put into SE:

$$i\hbar\partial_t \sum_n c_n(t)\,|\psi_n^{(0)}\rangle e^{-iE_n^{(0)}t/\hbar} = (H^{(0)} + V(t)) \sum_n c_n(t)\,|\psi_n^{(0)}\rangle e^{-iE_n^{(0)}t/\hbar}$$

$$\hookrightarrow i\hbar \sum_n \dot{c}_n(t)\,|\psi_n^{(0)}\rangle e^{-iE_n^{(0)}t/\hbar} = (H^{(0)} + V(t)) \sum_n c_n(t)\,|\psi_n^{(0)}\rangle e^{-iE_n t/\hbar}$$

$$+ \sum_n E_n^{(0)} c_n(t)\, e^{-iE_n^{(0)}t/\hbar}$$

$$\rightarrow \sum_n (i\hbar\partial_t c_n + E_n^{(0)} c_n)\,|\psi_n^{(0)}\rangle e^{-iE_n^{(0)}t/\hbar} = \sum_n (E_n^{(0)} + V(t))\, c_n\,|\psi_n^{(0)}\rangle e^{-iE_n^{(0)}t/\hbar}$$

multi. by bra...

$$\sum_n (i\hbar\partial_t c_n + E_n^{(0)} c_n)\,\delta_{mn}\, e^{-i(E_n^{(0)})t/\hbar} = \sum_n E_n^{(0)} c_n\, \delta_{mn}\, e^{-iE_n^{(0)}t/\hbar}$$

$$+ \sum_n \langle\psi_m^{(0)}|V(t)|\psi_n^{(0)}\rangle c_n e^{-iE_n^{(0)}t/\hbar}$$

$$\Rightarrow (i\hbar\partial_t c_m + E_m^{(0)} c_m)\, e^{-iE_m^{(0)}t/\hbar} = \langle\psi_m^{(0)}|V(t)|\psi_n^{(0)}\rangle c_n\, e^{-iE_n^{(0)}/\hbar}$$

↳ more legibly...

$$\boxed{(i\hbar\partial_t c_m + \cancel{E_m^{(0)} c_m})\, e^{-iE_m^{(0)}t/\hbar} = \sum_n \langle\psi_m^{(0)}|V(t)|\psi_n^{(0)}\rangle c_n\, e^{-iE_n^{(0)}t/\hbar}}$$

From there...

$$\partial_t c_m = \frac{-i}{\hbar} \sum_n \langle\psi_m^{(0)}|V(t)|\psi_n^{(0)}\rangle c_n\, e^{-i(E_n^{(0)} - E_m^{(0)})t/\hbar}$$

$$\hookrightarrow \boxed{\partial_t c_m = \frac{-i}{\hbar} \sum_n \overbrace{\langle\psi_m^{(0)}|V(t)|\psi_n^{(0)}\rangle}^{\text{mixed eigenstates}} c_n\, e^{-i\underbrace{(E_n^{(0)} - E_m^{(0)})}_{\Delta E}t/\hbar}}$$

Suppose we start out at $|i\rangle \Rightarrow$ pure state.

At $t=0 \Rightarrow c_i = 1$, $c_n = 0 \; \forall i$.

Then from $\partial_t c_m = \frac{-i}{\hbar}\sum_n \langle \psi_m^{(0)}|V(t)|\psi_n^{(0)}\rangle c_n e^{+i(E_m^{(0)}-E_n^{(0)})t/\hbar}$

we can integrate ... and look at c_f, of state $|f\rangle$

$$\partial_t c_f = \frac{-i}{\hbar}\sum_n \langle \psi_m^{(0)}|V(t)|i\rangle^{m} \overset{1}{c_i} e^{+i(E_f^{(0)}-E_i^{(0)})t/\hbar}$$

$$\partial_t c_f = \frac{-i}{\hbar}\langle f|V(t)|i\rangle e^{i(E_f^{(0)}-E_i^{(0)})t/t}$$

$$\boxed{c_f(t) = \frac{-i}{\hbar}\int_0^t (dt')\ \langle f|V(t')|i\rangle e^{i(E_f^{(0)}-E_i^{(0)})t'/\hbar}}$$

first-order approximation approximation ...

To get higher-order terms → put this back into the original equation → get higher order ...

Ex $V(t) = V_0 \cos(\omega t)$. Define $E_f^{(0)} - E_i^{(0)} = \hbar\omega_0$

freq of pert — natural freq ...

Then, $\langle f|V(t)|i\rangle = \cancel{E}\ \langle f|V_0\cos(\omega t)|i\rangle$

$$= \langle f|V_0|i\rangle \cos(\omega t)$$

$$= \langle f|V_0|i\rangle \left\{ \frac{1}{2}\left(e^{i\omega t} + e^{-i\omega t}\right) \right\}$$

So

$$c_f(t) = \frac{-i}{2\hbar}\int_0^t (dt')\ \langle f|V_0|i\rangle \left\{ e^{+i\omega t'} + e^{-i\omega t'} \right\} \left\{ e^{i\omega_0 t'} \right\}$$

(145)

Then $$c_f(t) = \frac{-i}{2\hbar}\int_0^t (dt')\, \langle f|V_0|i\rangle \left\{ e^{i(w+w_0)t} + e^{i(w_0-w)t} \right\}$$

$$= \frac{-i}{2\hbar} \langle f|V_0|i\rangle \int_0^t (dt') \left\{ e^{i(w+w_0)t} + e^{i(w_0-w)t} \right\}$$

$$\Rightarrow \boxed{c_f(t) = \frac{-1}{2\hbar}\langle f|V_0|i\rangle \left\{ \frac{e^{i(w_0+w)t}-1}{w_0+w} + \frac{e^{i(w_0-w)t}-1}{w_0-w} \right\}}$$

Case 1 $w_0 - w \simeq 0$, and $w_0 > 0$ $(E_f^{(0)} > E_i^{(0)})$ → 2nd term dom.

$$\boxed{c_f(t) = \frac{-1}{2\hbar}\langle f|V_0|i\rangle \frac{e^{i(w_0-w)t}-1}{w_0-w}}$$

Case 2 $w_0 < 0$ $(E_f^{(0)} < E_i^{(0)})$, $w \sim -w_0$ ... 1st term dominates

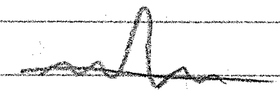
$$\boxed{c_f(t) = \frac{-1}{2\hbar}(f|V_0|i) \frac{e^{i(w_0+w)t}-1}{w_0+w}}$$ → same as before, only difference is sign ...

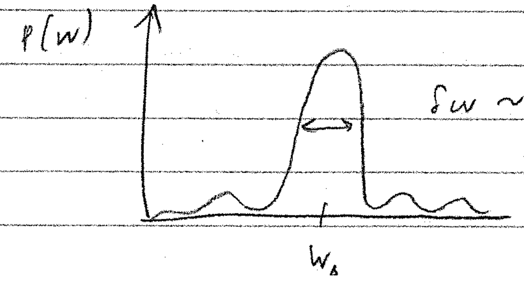
Transition probability → $P_{i\to f} = |c_f(t)|^2$

$$P_{i\to f} = |c_f(t)|^2 = \frac{1}{4\hbar^2}|\langle f|V_0|i\rangle|^2 \frac{1}{(w_0-w)^2} \underbrace{\left| e^{i(w_0-w)t} - 1\right|^2}$$

$$= \frac{1}{4\hbar^2}|\langle f|V_0|i\rangle|^2 \frac{1}{(w_0-w)^2}\, 4\sin^2\left(\frac{(w-w_0)t}{2}\right)$$

so $$\boxed{P_{i\to f} = \frac{|\langle f|V_0|i\rangle|^2}{\hbar^2} \sin^2\left(\frac{(w_0-w_0)t}{2}\right)\frac{1}{(w_0-w)^2}}$$





$\delta w \sim 1/t$

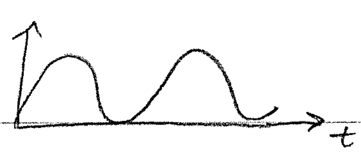
ec 2, 2019

$E = \hbar w$

$\delta E = \hbar \delta w \sim \hbar/t$

so $\boxed{t\,\delta E \sim \hbar}$ → need an energy range to get transition

<u>Note</u> $P_{i\to f}(t)$ osc in t



↳ If leave perturbation on, then at times

$t_n = \frac{2n\pi}{|\omega-\omega_0|}$ then system returns to its initial state.

$\Rightarrow$ $\boxed{\text{Rabi flopping}}$

↳ Rabi flopping freq: $\boxed{\omega_R = \frac{1}{2}\sqrt{(\omega-\omega_0)^2 + |\langle f|V_0|i\rangle/\hbar|^2}}$

//

EMISSION & ABSORPTION

- Atoms mostly interacts with $\vec{E}$ part of EM radiation.
- If λ of light is long compared to size of atom ($\sim$ Å) then we can treat $\vec{E}$ as spatially uniform.

↳ $\vec{E} = E_0 \cos(\omega t)\hat{k}$ → z-polarized

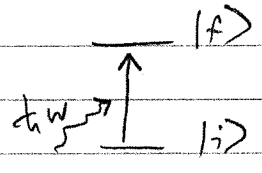
→ monochromatic, coherent source...

So, $\boxed{V(t) = -qE_0 z \cos(\omega t)}$

We already found transition probability...

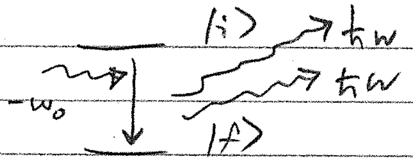
$$\boxed{P_{i\to f}(t) = \frac{1}{\hbar^2}\left|qE_0\langle f|z|i\rangle\right|^2 \frac{\sin^2((\omega-\omega_0)t/2)}{(\omega-\omega_0)^2}}$$

☒ If $E_i < E_f$



then atom <u>absorbs</u> a photon with $E_f - E_i = \hbar\omega$

☒ If $E_i > E_f$



, then atom emits a photon

$E_i - E_f = \hbar\omega$

Note probability of emission / absorption is same ...

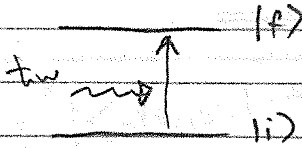
↳ how lasers work ... Atoms in an excited state, then start chain reaction ...

1 transition → $\hbar\omega$ → another transition ...
get chain reaction when majority of atoms are in excited states ...

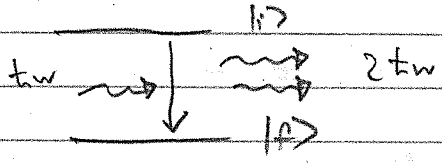
STIMULATED EMISSION

There's also SPONTANEOUS EMISSION (no $\bar{E}$ applied, but transition happens anyway)

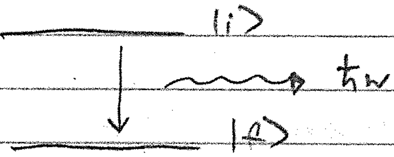
- Absorption:



- Stimulated emission



- Spontaneous emission



☒ what if we have an incoherent source?

If we have incoherent source of lots of frequencies ...

↳ then look at E density of an electric field ...

$$\boxed{u_{EM} = \frac{1}{2}\varepsilon_0 E_0^2} \rightarrow \left(\underline{\text{monochromatic...}}\right)$$

Energy density in a range of frequencies $d\omega$ is

$$\boxed{u \longrightarrow \int \rho(\omega)\,d\omega}.$$

<u>With this,</u>

$$\boxed{P_{i\to f}(t) = \frac{2q^2}{\varepsilon_0 \hbar}\left|\langle f|z|i\rangle\right|^2 \cdot \int_0^\infty \rho(\omega)\,\frac{\sin^2\left[(\omega_0-\omega)t/2\right]}{(\omega_0-\omega)^2}\,d\omega}$$

The $\frac{\sin^2 x}{x^2}$ is sharply peaked at $\omega_0 = \omega$, and $\rho(\omega)$ is broad...

↳ treat $\frac{\sin^2 x}{x^2}$ like a delta fn...

Also use $\int_{-\infty}^{\infty} \frac{\sin^2 x}{x^2}\,dx = \pi \rightarrow \int_0^\infty \frac{\sin^2 x}{x^2} = \frac{\pi}{2}$

$$\Rightarrow \boxed{P_{i\to f}(t) \cong \frac{\pi q^2}{\varepsilon_0 \hbar^2}\left|\langle f|z|i\rangle\right|^2 \rho(\omega_0)\,t}$$

Not osc in $t \Rightarrow$ no <u>flopping</u>... Transition rate

$R = \frac{dP}{dt}$ is constant $\boxed{R_{i\to f} = \frac{\pi q^2}{\varepsilon_0 \hbar^2}\left|\langle f|z|i\rangle\right|^2 \rho(\omega_0)}$

→ Now assume that light is randomly polarized...

<u>Then</u> look at $\left|q\langle f|\vec{r}|i\rangle \cdot \hat{n}\right|^2$ instead of $\left|\langle f|q^2 z|i\rangle\right|^2$

Want to average over all directions... By symmetry,...

$$\left|q\langle f|\vec{r}|i\rangle\right|^2 = \text{"}x^2\text{"} + \text{"}y^2\text{"} + \text{"}z^2\text{"} = 3\left|q\langle f|z|i\rangle\right|^2$$

With this, $\boxed{\left|q\langle f|\overset{\cdot\hat{n}}{\vec{r}}|i\rangle\right|^2_{\text{avg}} = \frac{1}{3}\left|q\langle f|\vec{r}|i\rangle\right|^2}$

And so, the transition rate for incoherent, unpolarized source is

$$\boxed{R_{i\to f} = \frac{\pi q^2}{3\epsilon_0\hbar^2}\left|\langle f|\vec{r}|i\rangle\right|^2\rho(\omega_0)}$$

dipole matrix element.

For hydrogen, $|i\rangle = |nlm\rangle$

$|f\rangle = |n'l'm'\rangle$

Dec 4, 2019

SELECTION RULES

From $R_{i\to f} = \frac{\pi q^2}{3\epsilon_0\hbar^2}\left|\langle f|\vec{r}|i\rangle\right|^2\rho(\omega_0)$

Since we're dealing with hydrogen... $|i\rangle = |nlm\rangle$

$\langle f| = \langle n'l'm'|$

a lot of the time $\langle f|\vec{r}|i\rangle = 0$. when?

■ Start with rules for m, Need info from L_z.

$$\left\{\begin{array}{lll} [L_z, x] & = L_z x - x L_z & = i\hbar y \\ [L_z, y] & = & = -i\hbar z \\ [L_z, z] & = & = 0 \end{array}\right\}$$

Now,

$$\langle n'l'm'|L_z\hat{x} - \hat{x}L_z|nlm\rangle = \hbar(m'-m)\langle n'l'm'|\hat{x}|nlm\rangle$$

So $= \boxed{i\cancel{\hbar}\langle n'l'm'|\hat{y}|nlm\rangle = \cancel{\hbar}(m'-m)\langle n'l'm'|\hat{x}|nlm\rangle}$

Similarly, $\boxed{-i\cancel{\hbar}\langle n'l'm'|\hat{x}|nlm\rangle = \cancel{\hbar}(m'-m)\langle n'l'm'|\hat{y}|nlm\rangle}$

→ 2 eqns, coupled... which give

$$(m'-m)\left\{ i(m'-m)\langle n'\ell'm'|y|n\ell m\rangle \right\} = i\langle n'\ell'm'|y|n\ell m\rangle$$

So $\quad (m'-m)^2 = 1 \Rightarrow \boxed{m' = m\pm 1}$

So we have $\boxed{\Delta m_\ell = \pm 1}$

and as by product... $\boxed{\langle n'\ell'm'|x|n\ell m\rangle = \pm i\langle n'\ell'm'|y|n\ell m\rangle}$

or m' = m, in which case ↗ = 0

With $[L_z, z]$,

$$\langle n'\ell'm'|\underbrace{L_z z - z L_z}_{[L_z, z]}|n\ell m\rangle = \hbar(m'-m)\langle n'\ell'm'|z|n\ell m\rangle = 0$$

$$\Rightarrow \boxed{m' = m}$$

So, selection rules for m: $\boxed{\Delta m = 0, \pm 1}$

$$\begin{cases} \Delta m = 0, & \text{then } \langle n'\ell'm'|x|n\ell m\rangle = \langle n'\ell'm'|y|n\ell m\rangle = 0 \\ \Delta m = \pm 1, & \text{then } \langle n'\ell'm'|x|n\ell m\rangle = \pm i\langle n'\ell'm'|y|n\ell m\rangle \end{cases}$$

and

$$\langle n'\ell'm'|z|n\ell m\rangle = 0$$

//

What about rules for ℓ? Use the commutator $[L^2, [L^2, \vec r]]$

- $[L^2, [L^2, \vec r]] = [L^2, L^2\vec r - \vec r L^2]$

prove...

$$\boxed{2\hbar^2(\vec r L^2 + L^2 \vec r) = L^2(L^2\vec r - \vec r L^2) - (L^2\vec r - \vec r L^2)L^2}$$

With this,

$$\langle n'\ell'm'|L^2(L^2\vec r - \vec r L^2)|n^{*}\ell^{*}m\rangle - \langle n'\ell'm'|(L^2 r - r L^2)L^2|n\ell m\rangle$$

$$= \hbar^2\{\ell'(\ell'+1) - \ell(\ell+1)\}\langle n'\ell'm'|L^2 r - r L^2|n\ell m\rangle$$

$$= [\hbar^2(\ell'(\ell'+1) - \ell(\ell+1))]^2\langle n'\ell'm'|\vec r|n\ell m\rangle$$

So, $\langle n'l'm'|\,[L^2,[L^2,\vec{r}]]\,|n\,l\,m\rangle = \boxed{\hbar^4\left[l'(l'+1) - l(l+1)\right]^2}\langle n'l'm'|\vec{r}|nlm\rangle$

$\Vert \qquad\qquad\qquad\qquad \Vert$

Also, $2\hbar^2\langle n'l'm'|\,L^2\vec{r}+\vec{r}L^2\,|n\,l\,m\rangle = \boxed{2\hbar^4\left(l'(l+1) + l(l+1)\right)}\langle n'l'm'|\vec{r}|nlm\rangle$

So, we need

$$\cancel{\hbar^4}\left[l'(l'+1) - l(l+1)\right]^2\langle n'l'm'|\vec{r}|nlm\rangle$$

$$= 2\cancel{\hbar^4}\left[l'(l'+1) + l(l+1)\right]\langle n'l'm'|\vec{r}|nlm\rangle$$

$$\left.\begin{array}{l}\text{So, either } \langle n'l'm'|\vec{r}|nlm\rangle = 0 \\ \quad\text{or } \left(l'(l'+1) - l(l+1)\right)^2 - 2\left(l'(l'+1) + l(l+1)\right) = 0\end{array}\right\}$$

$$\text{i.e. } \underbrace{(l'-l+1)\,(l'-l-1)}\;\underbrace{(l'+l)}_{\substack{\neq 0 \\ \text{since else} \\ \langle n'l'm'|\vec{r}|nlm\rangle = 0\ldots}}\;\underbrace{(l'+l+2)}_{\neq 0 \text{ since } l \geq 0} = 0$$

$$\downarrow$$

$$\boxed{\Delta l = \pm 1}$$

So, we've shown: $\boxed{\begin{array}{l}\Delta m = 0, \pm 1 \\ \Delta l = \pm 1\end{array}}$

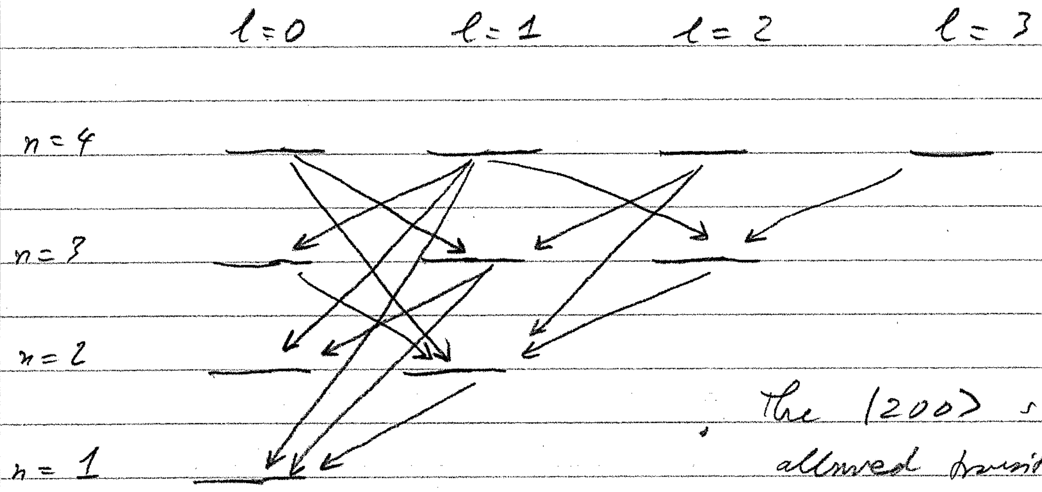
otherwise $\langle n'l'm'|\vec{r}|nlm\rangle = 0$ and $R_{i\to f} = 0$

Transitions that don't match these rules are forbidden...
↳ dipole transitions... For different kinds → might get different rules...

4

Level diagram through $n=4$ for hydrogen... ↘

(152)



- The $|200\rangle$ states have no allowed transitions to lower E.

↑ rules for dipole trans...

- Actually measured to have longer lifetime than $|21m_l\rangle$ states...

INTERPRETATION OF QM

Dec 5, 2019

① **Realist** Particles have properties that we can't determine b/c we don't have all the info.

"Hidden variables": Ψ is not the whole picture. There're some variables we just can't access

② **Orthodox** "Copenhagen interpretation" → determinacy is inherent in nature

③ **Agnostic** → Ignore problem.

Einstein-Podolski-Rosen Bohm Paradox
(EPR) (1935)

Consider decay of $\pi^0 \longrightarrow e^+ + e^-$. ~~[illegible]~~...
Pick frame such that

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$e^+ \leftarrow \pi^0 \rightarrow e^-$. Back-to-back decay to conserve momentum

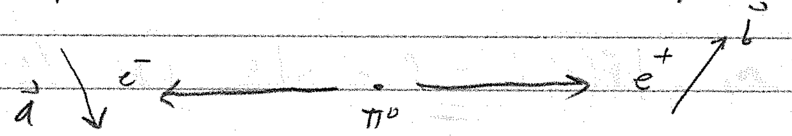
π^0 is spin 0, then $e^\pm$ are in singlet state: $\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$

Then, Stern-Gerlach: $\boxed{SG\hat{z}}\ e^+ \leftarrow \pi^0 \longrightarrow e^- \longrightarrow \boxed{SG\hat{z}}$

If e^- is $|\uparrow\rangle$ then e^+ is $|\downarrow\rangle$ and vice versa ...

↳ Bell's Inequality (1964)

Set up EPR-Bohm with random angle.



Measure spin at different angles ⇒ will always get $\pm\frac{\hbar}{2}$ (± 1)

☒ Look at average product: $P(\vec{a},\vec{b})$

$P(\vec{a},\vec{a}) = -1$ (regular EPR-Bohm)

$P(\vec{a},-\vec{a}) = +1$

so $\boxed{P(\vec{a},\vec{b}) = -\vec{a}\cdot\vec{b}}$

on any

☒ Assume some set of hidden variables λ

Result of e^-: $A(\vec{a},\lambda) = \pm 1$

Result of e^+: $B(\vec{b},\lambda) = \pm 1$

- If $\vec{a}=\vec{b}$ then $A(\vec{a},\lambda)B(\vec{b},\lambda) = -1$

$$\Rightarrow \quad A(\vec{a},\lambda) = -B(\vec{b},\lambda)$$

So, $P(\vec{a},\vec{b}) = \int \underset{\substack{\uparrow \\ \text{probability density}}}{\rho(\lambda)} A(\vec{a},\lambda)\, B(\vec{b},\lambda)\, d\lambda = -\int \rho(\lambda)\, A^{*}(\vec{a},\lambda)\, d\lambda$

$A(\vec{b},\lambda)$

- Consider a vector $\vec{c}$:

Then $P(\vec{a},\vec{b}) - P(\vec{a},\vec{c})$

$$= -\int \rho(\lambda)\left\{ \vec{A}(\vec{a},\lambda)\vec{A}(\vec{b},\lambda) - A(\vec{a},\lambda)\,A(\vec{c},\lambda)\right\} d\lambda$$

Because $A^2(\vec{b},\lambda) = +1$,

$$P(\vec{a},\vec{b}) - P(\vec{a},\vec{c}) = -\int \rho(\lambda)\left\{1 - A(\vec{b},\lambda)A(c,\lambda)\right\} A(\vec{a},\lambda)A(\vec{b},\lambda)\,d\lambda$$

now, $\left|A(\vec{a},\lambda)A(\vec{b},\lambda)\right| = 1$ and

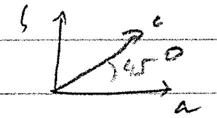
$$\rho(\lambda)\left(1 - A(\vec{b},\lambda)A(\vec{c},\lambda)\right) \geq 0 .$$

And so, $\left|\vec{P}(\vec{a},\vec{b}) - P(\vec{a},c)\right| \leq \int \rho(\lambda)\left(1 - A(\vec{b},\lambda)A(\vec{c},\lambda)\right) d\lambda$

which means

$$\boxed{\left|P(\vec{a},\vec{b}) - P(\vec{a},\vec{c})\right| \leq 1 + P(\vec{b},\vec{c})}$$ ⇝ if λ exists...

Look at ...



$P(\vec{a},\vec{b}) = 0$

$P(\vec{b},\vec{c}) = P(\vec{a},\vec{c}) = \frac{-1}{\sqrt{2}}$

But $\underbrace{\left|0 - \left(\frac{-1}{\sqrt{2}}\right)\right|}_{} \leq 1 + \left(\frac{-1}{\sqrt{2}}\right)$

$0.707 \leq 0.293$ ... ⇒ contradiction...

So, hidden variable λ is incompatible with QM...

{Schrödinger's Cat} (1935)

$$\psi_{cat} = \frac{1}{\sqrt{2}}\left(\psi_{alive} + \psi_{dead}\right)$$

{Wigner's friend}

$|1\rangle$ = particle $|\uparrow\rangle$, friend sees $|\uparrow\rangle$

$|2\rangle$ = particle $|\downarrow\rangle$, friend sees $|\downarrow\rangle$

But when does measurement occur?

$\boxed{\text{Interpretations}}$ What is a measurement?

① **Wigner**: intervention of human consciousness.

② **Bohr**: Interaction between quantum system + macroscopic measurement apparatus

③ **Heisenberg** when permanent record is left

④ Measurement happens when sth irreversible occurs.

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ec 6, 2019

$\boxed{\text{REVIEW}}$

Time independent Pert. Theory $H = H^{(0)} + H'$

⊡ First correction: $E^{(1)} = \langle n | H' | n \rangle$

non-degenerate

$$\psi_n^{(1)} = \sum_{m \neq n} \frac{\langle m | H' | n \rangle}{E_n^{(0)} - E_m^{(0)}} | m \rangle$$

$$\psi_n = \psi_n^{(0)} + \psi_n^{(1)} + \ldots$$

⊡ Second order correction:

$$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle m | H' | n \rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

Degenerate ⊡ If states have same energy but are still orthogonal

First order correction $H'_{ij} = \langle i | H' | j \rangle$

- if diagonal, then states are eigenstates. corrections are diagonal entries...

- if not diagonal, then must find eigen val, eigenvec for the matrix.

☐ If H' doesn't mix degenerate states (diagonal) then second order can be found via

$$E^{(2)} = \sum_{m \neq n} \frac{|\langle m|H'|n\rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

where $\langle m|$ is <u>not</u> one of the degenerate states.

☐ <u>Hydrogen structure</u> $\boxed{\text{fs} = \text{rel} + \text{s.o}}$ → good states $|n\, j\, m_j\rangle$

$\boxed{\text{Zeeman} = \frac{e}{2m}(\vec{L} + 2\vec{S})\cdot\vec{B}_{ext}}$ → good states $|n\, l\, m_l\, m_s\rangle$

$\boxed{\text{Hf} = \text{spin-spin}}$ $\vec{S}_e \cdot \vec{S}_p$.

↳ good state: total spin $\vec{S} = \vec{S}_e + \vec{S}_p$