(first-order, time independent)

(9) Perturbation Theory

[A way to deal with complicated problems if we get approximate like a near simple one. Here we'll do just first-order correction and time independent problem (but can be extended beyond both of these).]

$\hat{H} = \hat{H}_0 + \hat{H}'$ write as $\hat{H} = \hat{H}_0 + \lambda \hat{H}_1$, to keep track of smallness.

Deals with systems that have a Hamiltonian: $\hat{H} = \hat{H}_0 + \lambda \hat{H}_1$

where $\hat{H}_0$ is a simple problem that can be easily solved exactly

$$\hat{H}_0 |\varphi_n\rangle = E_n^{(0)} |\varphi_n\rangle$$

[Comment on Dirac notⁿ: φ_n could be 1 electron or 6 million and don't want to write that down]

Use these eigenfunctions to solve the full problem:

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

If λ is small (i.e. a perturbation!) expand E_n and $|\varphi_n\rangle$ as series:

$$E_n \sim E_n^{(0)} + \lambda E_n^{(1)}$$

$$|\psi_n\rangle \sim |\varphi_n\rangle + \lambda \sum_{m \neq n} c_{nm} |\varphi_m\rangle$$

small admixtures of other eigenfunctions

keep series to first order i.e. neglect λ^2 and higher

[Try to get the shift in energy $\lambda E_n^{(1)}$]

[reinforce that perturbation mixes φ_m for use later in lecture]

Sub into LHS of TISE:

$$\hat{H} |\psi_n\rangle = \left(\hat{H}_0 + \lambda \hat{H}_1\right)\left(|\varphi_n\rangle + \lambda \sum_{m \neq n} c_{nm} |\varphi_m\rangle\right)$$

$$= \hat{H}_0 |\varphi_n\rangle + \lambda \sum_{m \neq n} c_{nm} \hat{H}_0 |\varphi_m\rangle + \lambda \hat{H}_1 |\varphi_n\rangle + \text{terms in } \lambda^2$$

$$= E_n^{(0)} |\varphi_n\rangle + \lambda \sum_{m \neq n} c_{nm} E_m^{(0)} |\varphi_m\rangle + \lambda \hat{H}_1 |\varphi_n\rangle$$

and RHS:

$$E_n|\psi_n\rangle = \left(E_n^{(0)} + \lambda E_n^{(1)}\right)\left(|\varphi_n\rangle + \lambda \sum_{m\neq n} c_{nm}|\varphi_m\rangle\right)$$

$$= E_n^{(0)}|\varphi_n\rangle + \lambda E_n^{(1)}|\varphi_n\rangle + \lambda E_n^{(0)} \sum_{m\neq n} c_{nm}|\varphi_m\rangle + \text{terms in } \lambda^2$$

Equate and tidy up (first terms above cancel)

$$\lambda E_n^{(1)}|\varphi_n\rangle + \lambda \sum_{m\neq n} (E_n^{(0)} - E_m^{(0)}) c_{nm}|\varphi_m\rangle = \lambda \hat{H}_1|\varphi_n\rangle \quad (1)$$

Now overlap with $\langle\varphi_n|$ [i.e. multiply by φ_n^* and integrate over all coords]

$$\lambda E_n^{(1)} \underbrace{\langle\varphi_n|\varphi_n\rangle}_{=1} + \lambda \sum_{m\neq n} (E_n^{(0)} - E_m^{(0)}) c_{nm} \underbrace{\langle\varphi_n|\varphi_m\rangle}_{=0} = \lambda \langle\varphi_n|\hat{H}_1|\varphi_n\rangle$$

KEEP

Assumed $|\varphi_n\rangle$ is normalised $\langle\varphi_n|\varphi_n\rangle = 1$
and eigenstates are orthogonal $\langle\varphi_n|\varphi_m\rangle = 0$ if $n\neq m$

$$\lambda E_n^{(1)} = \lambda \langle\varphi_n|\hat{H}_1|\varphi_n\rangle = \lambda \int \varphi_n^*(\underline{r}) \hat{H}_1 \varphi_n(\underline{r})\, d^3\underline{r}$$

(for one particle state)

So to first order in λ, the shift in an eigenvalue is just the expectation value of the perturbation, using the unperturbed eigenstates.

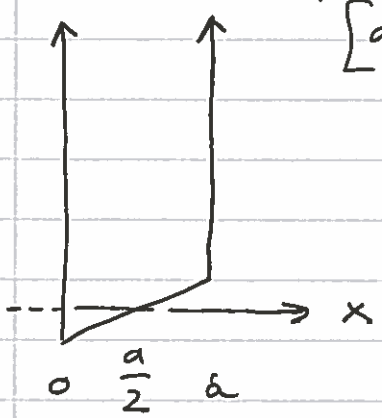
$$\delta E_n = \lambda E_n^{(1)} = \langle \lambda \hat{H}_1 \rangle = \langle \hat{H}' \rangle$$

i.e. if perturbation is small, original eigenstates don't change much, so the change in energy is just the average value of the perturbation.

CAN FAIL THOUGH! (See below)

Example: in our quantum dot we'd neglected the tilted floor!
unperturbed: electron in infinite square well
added electric field $\mathcal{E}$.

[adjust gate so V=0 in middle]



$$V(x) = e\mathcal{E}\left(x - \frac{a}{2}\right) \quad 0 < x < a$$
$$\infty \quad \text{outside}$$

Unperturbed: infinite sq well $\quad \varphi_n(x) = \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a}$

[NB: eigenfunctions are normalised – essential!] $\quad E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2} \quad n = 1, 2, \ldots$

Perturbation: $\hat{H}' = e\mathcal{E}\left(x - \frac{a}{2}\right)$

$$\delta E_n = \langle \varphi_n | \hat{H}' | \varphi_n \rangle = \int_0^a \varphi_n^*(x) V(x) \varphi_n(x)\, dx$$

$$= \frac{2}{a} e\mathcal{E} \int_0^a \left(x - \frac{a}{2}\right) \sin^2 \frac{n\pi x}{a}\, dx \quad \text{and integrate}$$

$\left(x - \frac{a}{2}\right)$: odd function about $x = a/2$

$\sin^2 \frac{n\pi x}{a}$: even function about $x = \frac{a}{2}$

$$= 0 \quad \text{since product is odd.}$$

So to first order no effect of a tilted bottom.
[did the right thing ignoring it]
Need to calculate corrections to second order ie. $\mathcal{E}^2$ to see an effect.

[if your bottom is tilted, don't worry about it – at least to first order]

To find the new wavefunctions, need to find the expansion coefficients, so go back to eq^n ① and overlap with $\langle \varphi_k |$ when $k \neq n$ and use orthogonality:

$$\lambda (E_n^{(0)} - E_k^{(0)}) c_{nk} = \lambda \langle \varphi_k | \hat{H}_1 | \varphi_n \rangle$$

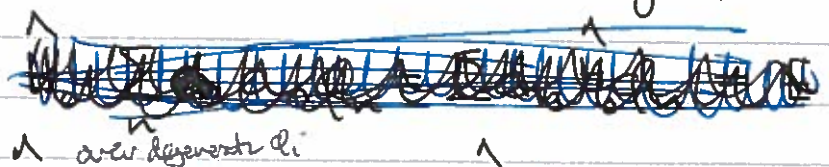
two indices n & k so like the element of a 2×2 matrix

ie. calculate the integral (or matrix element) on LHS and divide by $\lambda (E_n^{(0)} - E_k^{(0)})$ // But if this is ZERO you have a problem!

new line

This will arise if $\hat{H}_0$ has degenerate eigenstates.

But in degenerate case any linear combination of degenerate eigenfunctions is also an eigenfunction:



or refer to RAE and 2nd year

over degenerate φ_i

$$\hat{H}_0 \sum_i a_i |\varphi_i\rangle = \sum a_i \hat{H}_0 |\varphi_i\rangle = E \sum a_i |\varphi_i\rangle$$

So, choose some combination that doesn't get mixed by $\hat{H}_1$, ie. $\langle \varphi_k | \hat{H}_1 | \varphi_n \rangle = 0$ if $E_n^{(0)} = E_k^{(0)}$ $n \neq k$

Then calculate δE as above. (see Rae 7.2)

[Techniques associated with "matrix diagonalisation" can be extended to situations where perturbations are not small → but outside our remit.]

$$\nabla^2\psi = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial \psi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\varphi^2} + \frac{\partial^2\psi}{\partial z^2}$$

cylindrical polars.

(10) Quantum Wires and Nanotubes

Deal with long narrow wires where width of conductor is small enough to expect quantal behaviour

electrons in

H splits into z and φ components, giving electron energies: $E = \frac{\hbar^2 k_z^2}{2m^*} + E_{xy}$

E_{xy} ← eigenvalue of xy motion [depends on details of size and shape]

↑ ie. no potential in z

$E = \frac{p^2}{2m}$ for free particle

remember m^* is reduced mass mopping up some of effects of interactions

In the z-direction:

sinusoidal ψ as no potential in z

$L = n\frac{\lambda}{2}$

$k = \frac{2\pi}{\lambda}$

If ends are insulating: wavefunction vanishes at $z=0$ and $z=L$

and $k_z = \frac{n\pi}{L}$ $n = 1, 2, \ldots$ [choice of BCs doesn't matter if L is very long]

Plotted against k_z, the states are evenly spaced:

How many states in region $k_z \to k_z + \delta k_z$?

$$\frac{\delta k_z}{\pi/L} \times 2 = \frac{2L}{\pi}\delta k_z$$

factor of two for spin up/down

If L very large $\delta k_z \to dk_z$: $\#\text{states} = \frac{2L}{\pi}dk_z$

$$\frac{dn}{dk_z} = \frac{2L}{\pi}$$ "density of states"

In terms of energy $k_z = \sqrt{\frac{2m^*}{\hbar^2}(E - E_m)}$

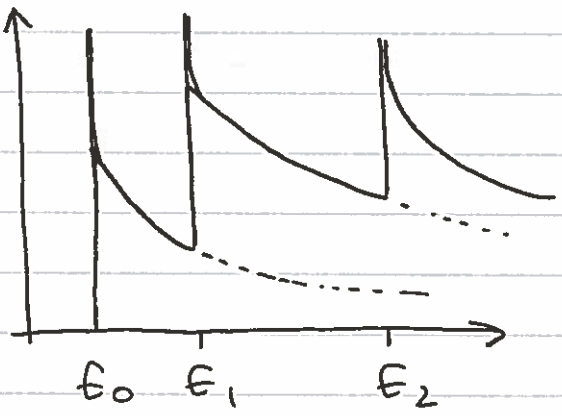
$$\frac{dk_z}{dE} = \left(\frac{2m^*}{\hbar^2}\right)^{1/2} \cdot \frac{1}{2} \cdot \frac{1}{\sqrt{(E - E_m)}}$$

So for electrons in a particular x_y state:

$$\frac{dn}{dE} = \frac{dn}{dk_z} \cdot \frac{dk_z}{dE} = \frac{L}{\pi} \cdot \left(\frac{2m^*}{\hbar^2}\right)^{1/2} \cdot \frac{1}{\sqrt{E - E_m}}$$

density of states in 1D.

Overall the numbers of states from different E_m add up:



sharp spikes at energies E_m (van Hove singularities)

very different from a bulk conductor

[In 3D bulk $\frac{dn}{dE} \propto \sqrt{E}$

smooth with E]] mark to

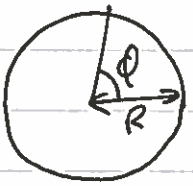
different as electron is "trapped" in the $r\varphi$ plane to finite region.

Circular sym so best to use (r, θ) usual now separate into radial + angular eq^{n}s

In the $r\varphi$ plane:

turns out that radial excitations are several eV (ignore here)

esp. for thin walled tubes confined to R



angular TISE:

$$-\frac{\hbar^2}{2m^*R^2}\frac{d^2\psi}{d\varphi^2} = E\psi$$

$\leftrightarrow$ moment of inertia

$$\frac{d^2\psi}{d\phi^2} = -p^2\psi \quad \text{when} \quad p^2 = \frac{2m^*R^2E}{\hbar^2}$$

fitting a periodic function around

Solution: $\psi = Ae^{ip\varphi}$

Boundary condition: $\psi(\varphi) = \psi(\varphi + 2\pi)$
periodic

$\Rightarrow p$ must be an integer

Eigenvalues are: $E_0 = 0$
$E_1 = \hbar^2/2m^*R^2$
$E_2 = 4\hbar^2/2m^*R^2$
$\vdots$
} doubly degenerate due to spin.

Expect spikes in conductance when potential driving current is such that electron energy matches one of these due to the large density of states available to carry the current.

(*)

What nanotubes are available to check?

(i) silicon/germanium nanowires: conducting cylinders with walls an atom thick.
important as could improve capacity of Li-ion batteries by increasing electrode area

$R \sim 20\,nm \quad m^* = 0.2m_e \quad E_1 = \frac{\hbar^2}{2m^*R^2} \sim 4.75 \times 10^{-4}$ eV

→ too small to resolve.

(ii) carbon nanotubes "discovered" 1991 (had been seen in soot years before!)

sheet of graphene rolled up into a tube.

but the effective mass of electrons in graphene turns out to be zero!

$m^x = 0$ → rather like relativistic particles.

Limiting velocity is $V_F \sim 10^6 ms^{-1}$ (cf speed of light)

"Relativistic" energy $\epsilon = V_F|p|$ cf $\epsilon = cp$

$= \hbar V_F |\underline{k}|$

For the angular wavefunction application of periodic boundary conditions gives

$\lambda = \frac{2\pi R}{n}$ n = integer

[$L = n\lambda/2$
$\lambda = 2\pi/k$]

$k = \frac{2\pi}{\lambda} = \frac{n}{R}$

So this time $\epsilon_n = \frac{\hbar V_F}{R} n$ where $R \sim 0.7nm$

→ equally spaced spikes in conductance not 1:4:9....

$\epsilon_1 = \hbar c \frac{V_F}{c} \frac{1}{R} = 197 \times \frac{1}{300} \times \frac{1}{0.7}$

$= 0.94 eV$

[

(11) Angular Momentum

Quick recap from 20101:

Position and momentum are incompatible observables - can't know both simultaneously

Signature: their operators don't commute

$\hat{p}_x = i\hbar \frac{\partial}{\partial x}$ $\quad \hat{x} = x$ $\quad [\hat{p}_x, \hat{x}] = \hat{p}_x\hat{x} - \hat{x}\hat{p}_x = -i\hbar$

and similar for y and z.

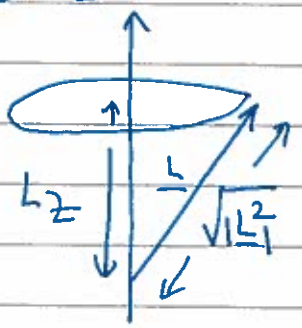
Orbital ang. mom: $\underline{\hat{L}} = \underline{\hat{r}} \times \underline{\hat{p}}$ $\quad \hat{L}_x = y\hat{p}_z - z\hat{p}_y$ and cyclically then $x \to y \to z$

Components do not commute: $[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$ and cyc

but they do commute with $\hat{L}^2$: $[\hat{L}^2, \hat{L}_z] = 0$

So the most we can know is the ~~length~~ (or $|\underline{L}|^2$) and one component, say L_z. z

Picture:



know: length and z-component of $\hat{\underline{L}}$ and $\hat{L}_z$ same eigenfunc.

L_x and L_y uncertain; end of $\underline{L}$ lies anywhere on circle

Must have: $|\underline{L}|^2 \geq L_z^2$

In Paths20101

Write operators as differential form and solve eigenfunctions:

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

$$\hat{L}_z Y_{lm}(\theta,\phi) = m\hbar Y_{lm}(\theta,\phi)$$

l integer ≥ 0

$-l \leq m \leq l$

m: integer

Y_{lm}: Spherical harmonics

Try something more general — do operators need to be differential operators?

Eigenvalue eqⁿs: $\hat{L}^2\phi = \alpha\phi$ * $\quad \hat{L}_z\phi = \beta\phi$ * $\quad \alpha \geq \beta^2$

what are α, β and ϕ?

Define two new operators: $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$ called ladder operators

We'll need to know products: [be careful of order]

$$\hat{L}_+\hat{L}_- = \hat{L}_x^2 + \hat{L}_y^2 - i[\hat{L}_x, \hat{L}_y]$$
$$= \hat{L}^2 - \hat{L}_z^2 + \hbar\hat{L}_z \quad *$$

Similarly $\hat{L}_-\hat{L}_+ = \hat{L}^2 - \hat{L}_z^2 - \hbar\hat{L}_z$ * $\Big\}$ $[\hat{L}_+, \hat{L}_-] = 2\hbar\hat{L}_z$

Other commutators:

$$[\hat{L}_z, \hat{L}_+] = [\hat{L}_z, \hat{L}_x] + i[\hat{L}_z, \hat{L}_y]$$
$$= i\hbar(\hat{L}_y - i\hat{L}_x) = \hbar\hat{L}_+ \quad *$$

and similarly $[\hat{L}_z, \hat{L}_-] = -\hbar\hat{L}_-$ *

Also $\hat{L}^2$ commutes with $\hat{L}_{x,y}$ $\rightarrow$ $[\hat{L}_\pm, \hat{L}^2] = 0$ *

Now for you operate on the L_z eigenvalue eqⁿ:

$$\hat{L}_+\hat{L}_z\phi = \hat{L}_+\beta\phi$$
$$(\hat{L}_z\hat{L}_+ - \hbar\hat{L}_+)\phi = \beta\hat{L}_+\phi$$
$$\hat{L}_z\hat{L}_+\phi = (\beta+\hbar)\hat{L}_+\phi$$

eigenfunction!

$\hat{L}_+\phi$ looks like a new eigenfunction of $\hat{L}_z$ with eigenvalue $\beta+\hbar$. (NB, it isn't normalised)

If you use L_- instead, show that

$$\hat{L}_z\hat{L}_-\phi = (\beta-\hbar)\hat{L}_-\phi$$

$\hat{L}_\pm\phi$ is a new eigenfunction of $\hat{L}_z$ with eigenvalue $\beta\pm\hbar$

(but it isn't normalised).

Rungs separated by $\hbar$: $p_1 - p_2 = n\hbar$ n = positive integer.

$p_1 - (-p_1) = n\hbar$

Top rung $p_1 = \frac{n\hbar}{2}$ Bottom $p_2 = -\frac{n\hbar}{2}$

ie. $-\frac{n\hbar}{2} \leq p \leq \frac{n\hbar}{2}$ in steps of $\hbar$

And $\alpha = p_1(p_1+\hbar) = \frac{n\hbar}{2}\left(\frac{n\hbar}{2}+\hbar\right) = \hbar^2 \frac{n}{2}\left(\frac{n}{2}+1\right)$

So got eigenvalues without solving eigenvalue eq^n — NEAT.

If n is an even integer:

$\alpha = \hbar^2 l(l+1)$ l integer $\quad -l\hbar \leq p \leq l\hbar$ $m\hbar$

] just what we had in 20101 with nice eigenfunctions $Y_{lm}(\theta, \phi)$

but something new if, n is odd integer!

Implies possibility of ang mom being a half integer.

Eg $\frac{n}{2} = \frac{1}{2}$ $\alpha = \hbar^2 \frac{3}{4}$ $p = -\frac{\hbar}{2}$ or $+\frac{\hbar}{2}$

Two ways to orientate

$\Rightarrow$ spin up / down ?

Exactly what is need to describe intrinsic spin.

But what are the eigenfunctions?

Two types of ang. mom: orbital and intrinsic spin

cf classically orbiting planet, spinning on its axis.

But in QM no evidence of anything literally spinning.

[Mechanical version of electron needs rotation so just a point on the surface requires speeds greater than c — but it has no "size" anyway so how could it spin!]

If you do the same to the $\hat{L}^2$ eigenvalue eqn:

$$\hat{L}_\pm \hat{L}^2 \phi = \hat{L}_\pm \alpha \phi$$

$$\hat{L}^2 \hat{L}_\pm \phi = \alpha \hat{L}_\pm \phi$$

as $[\hat{L}_+, L^2] = 0$.

So $\hat{L}_\pm \phi$ are still eigenfunctions of $\hat{L}^2$.

So $\hat{L}_\pm$ raise and lower the eigenfunctions up and down a "ladder" of $\hat{L}_z$ eigenvalues (β) corresponding to the $\hat{L}^2$ eigenvalue (α), which rungs are separated by $\hbar$.
But if $\beta^2 \leq \alpha$ there are max and min values β_1 and β_2 and corresponding eigenfunctions ϕ_1 and ϕ_2. at top + bottom.

At the top of the ladder, can't raise anymore: $\hat{L}_+ \phi_1 = 0$
and at the bottom, can't lower: $\hat{L}_- \phi_2 = 0$

Take the first and operate with $\hat{L}_-$

$$\hat{L}_- \hat{L}_+ \phi_1 = \left(\hat{L}^2 - \hat{L}_z^2 - \hbar \hat{L}_z\right) \phi_1 = \left(\alpha - \beta_1^2 - \hbar \beta_1\right) \phi_1 = 0$$

So $\alpha = \beta_1 (\beta_1 + \hbar)$

Similarly:

$$\hat{L}_+ \hat{L}_- \phi_2 = \left(\hat{L}^2 - \hat{L}_z^2 + \hbar \hat{L}_z\right) \phi_2 = \left(\alpha - \beta_2^2 + \hbar \beta_2\right) \phi_2 = 0$$

$$\alpha = \beta_2 (\beta_2 - \hbar)$$

$$\beta_1 (\beta_1 + \hbar) = \beta_2 (\beta_2 - \hbar)$$

Satisfied if $\beta_2 = -\beta_1$ ie. rungs are symmetric about zero. (max/min)
(NB // $\beta_2 < \beta_1$)

(12) Intrinsic Spin

Now have possibility of $\frac{n}{2}$-spin where n is odd integer.

Spin-1/2 is special

Dirac showed QM + relativity ⇒ electron is a point particle with a property that behaves like a half-integer angular momentum.

[You could read about Dirac's theory in Rae – but not part of this course.]

Experimentally:

particles that are not spin-1/2 are either composite objects or are mysterious exchange particles like the photon (see Mitch's course).

Okay what about the eigenfunctions? Without the l integer condition were regular spatial functions want do!

Have orthonormalisation $\int \psi_i^* \psi_j \, dV = \delta_{ij}$

expectation $\langle O \rangle = \int \psi_i^* \hat{O} \psi_i \, dV$

1927 Phipps Taylor: neutral H beam splits into 2 components in a magnetic field. except $L=0$!

(12) Intrinsic Spin exemplified by Electrons.

Something missing in early QM: Na atoms in magnetic fields split into even # of states if integer except odd #

Twice the expected # of electrons in atomic shells

1925

Worthy an exp. of fine structure of atomic lines crack the problem; two Postdocs Sam Goudsmit, George Uhlenbeck } electron has intrinsic spin $\hbar/2$

Saw this arise from ladder ops; now concentrate on electrons. use S when talking about spin.

We've deduced the eigenvalues of $\hat{S}^2$ and S_z:

$$\hat{S}^2 \chi = \hbar^2 s(s+1)\chi = \frac{3}{4}\hbar^2 \chi$$

$$\hat{S}_z \chi = m_s \hbar \chi = \pm \frac{1}{2}\hbar \chi$$

What about eigenfunctions?

so-called "up" and "down" [Dangerous! really the z comp is up or down.

No spatial wavefunction has the right properties: integer ang. mom. required.

Forced into a different mathematical language.

Simplest choice is to use vectors. (Columns)

$$m_s = +\frac{1}{2} \rightarrow \alpha_z \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad m_s = -\frac{1}{2} \rightarrow \beta_z \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

These are examples of things called "spinors" (spin vectors). Sometimes α_z and β_z if need to make axis of quantn clear.

[How are these things orthogonal?] $\int \psi_i^* \psi_j \, dV = \delta_{ij}$

Scalar product for spinors: $\alpha_z^\dagger \alpha_z = (1 \; 0) \begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1$ so normalised

This is a transposed, complex conjugate "Hermitian conjugate"

1921: Compton notes oblique ref to spinning electrons

1927: neutral H beam in SG expt Phipps and Taylor
$L=0$ splits in 2.
Can't be nuclear effect $\frac{e\hbar}{2m}$

Ignore 2016.

1925: Goudsmit and Uhlenbeck graduate students (Sommerfeld relativistic electron orbits charge with velocity).
waiting on fine structure
electron spin $\pm\frac{\hbar}{2}$
noted in H not alkalis.

Issues: difference in mass/charge distn leads to $g \neq 1$.
$g_s = 2$ from sphere of charge with charge on surface
↳ needed velocity at surface of electron faster than c.
all sorts of other electrodynamic issues with a literally spinning electron.

They became sceptical, but their boss had already submitted their paper for them

"I have already sent your letter in but you are both young enough to allow yourselves some foolishness".

$\beta_z^+ \alpha_z = (0\ 1)\begin{pmatrix}1\\0\end{pmatrix} = 0$ ie. orthogonal.

or if you like to combine the two properties "orthonormal".

Just like expanding a wave function in a basis set of eigenfunctions, can form a general spinor:

$$\chi = c_1 \alpha_z + c_2 \beta_z = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

where c_1 and c_2 are in general complex.

Normalised if: $\chi^+ \chi = (c_1^* \; c_2^*)\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 1$

ie. $|c_1|^2 + |c_2|^2 = 1$

↑ ↑ — looking like probabilities of "up" and "down"

[So we're getting towards a full "spin algebra". Have eigenvalues, eigenfunctions, but need some operators:]

In order for it to work as an ang. mom need to satisfy:

$[\hat{S}_x, \hat{S}_y] = i\hbar \hat{S}_z$ and $[\hat{S}^2, \hat{S}_z] = 0$ and cyclically.

But what operates on a vector?

Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

[Matrix multiplication: product elements are the scalar products of the defining row and column]

Some quick checks... products.

$$\sigma_1\sigma_2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = i\sigma_3$$

$$\sigma_2\sigma_1 = \qquad\qquad = -i\sigma_3$$

} order of product matter.

$[\sigma_1, \sigma_2] = \sigma_1\sigma_2 - \sigma_2\sigma_1 = 2i\sigma_3$ ie. looks like angular mom but missing an $\hbar$ and has factor 2.

Define:

$$\hat{S}_x = \frac{\hbar}{2}\sigma_1 \qquad \hat{S}_y = \frac{\hbar}{2}\sigma_2 \qquad \hat{S}_z = \frac{\hbar}{2}\sigma_3$$ to satisfy normal commutators.

But are the eigenvalues/vectors right?

$$\hat{S}_z\alpha = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}\alpha$$ ← eigenfunction; ← eigenvalue

$$\hat{S}_z\beta = \qquad\qquad = -\frac{\hbar}{2}\beta$$

The squares of the matrices are all the same:

$$\hat{S}_x^2 = \hat{S}_y^2 = \hat{S}_z^2 = \frac{\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$ ← identity matrix!

So $\hat{S}^2 = \frac{3\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \rightarrow \hat{S}^2 \propto \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ so must commute with $\hat{S}_x$, $\hat{S}_y$ and $\hat{S}_z$

and also $\hat{S}^2 \chi = \frac{3}{4}\hbar^2 \chi$ for $\chi = c_1\alpha_z + c_2\beta_z = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$

↑ eigenvalue $= \frac{3}{4}\hbar^2 = \frac{1}{2}\left(\frac{1}{2}+1\right)\hbar^2$

If you are in a state described by χ:

$$\langle \hat{S}_z \rangle = \chi^+ \hat{S}_z \chi = \frac{\hbar}{2}(c_1^* c_2^*)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

$$\left[\langle O \rangle = \int \psi_i^* \hat{O} \psi_i \, dV\right] = \frac{\hbar}{2}|c_1|^2 - \frac{\hbar}{2}|c_2|^2$$

↑ ↑

so these are probabilities of "up" and "down".

How would you find spinors for quantisation along x axis?

Solve eigenvalue eqn: $\sigma_1 \frac{\hbar}{2}\begin{pmatrix} u \\ v \end{pmatrix} = \lambda \begin{pmatrix} u \\ v \end{pmatrix}$

↑ eigenvalue.

[deal with $\hbar/2$ later!]

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} = \lambda \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix}$$

↳ λ times identity.

$$\Rightarrow \begin{pmatrix} -\lambda & 1 \\ 1 & -\lambda \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} = 0$$

either $u = v = 0$

or $\begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} = 0$

$\Rightarrow \lambda^2 - 1 = 0 \quad \lambda = \pm 1$ So eigenvalues of $\hat{S}_x = \pm\frac{\hbar}{2}$

if $\lambda = +1$: $-u + v = 0$

$v = u$ $\Big\}$ $\alpha_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

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if $\lambda = -1$: $u + v = 0$, $v = -u$ $\Rightarrow \beta_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$

A complete spinor wavefunction for, say, an electron:

$$\psi(\underline{r}) = \psi_1(\underline{r})\alpha_z + \psi_2(\underline{r})\beta_z$$

$$= \begin{pmatrix} \psi_1(\underline{r}) \\ \psi_2(\underline{r}) \end{pmatrix}$$

Prob of finding electron of spin "up" at $\underline{r}$ $= |\psi_1(\underline{r})|^2$

and spin "down" at $\underline{r}$ $= |\psi_2(\underline{r})|^2$

Normalised if $\int \psi^+(\underline{r})\,\psi(\underline{r})\,d^3\underline{r} = \int |\psi_1(\underline{r})|^2 + |\psi_2(\underline{r})|^2 d^3\underline{r} = 1$