

XPHC 2663 / XPHA 2663

SECOND PUBLIC EXAMINATION

Honour School of Physics Part A: 3 and 4 Year Courses

Honour School of Physics and Philosophy Part A

A3: Quantum Physics

Friday, 20 June 2003, 9.30 am – 12.30pm

Answer all of Section A and three questions from Section B.

Start the answer to each question on a fresh page.

A list of physical constants and conversion factors accompanies this paper.

The numbers in the margin indicate the weight which the Examiners expect to assign to each part of the question.

Do NOT turn over until told that you may do so.

$$\begin{pmatrix} \zeta & -\zeta \\ \zeta & \zeta \end{pmatrix} \begin{pmatrix} 1 \\ i \end{pmatrix} \Rightarrow \begin{pmatrix} \zeta \\ i \end{pmatrix} \cdot \begin{pmatrix} 1 \\ i \end{pmatrix} \not\propto .$$

Section A

1. Explain which aspects of the *photo-electric effect* cannot be accounted for by classical physics and how Quantum Theory resolves the difficulties. [7]

2. Show that the matrices

$$s_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad s_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad s_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

satisfy the commutation rules for angular momentum. Find the eigenvalues and normalized eigenvectors of s_x . [8]

3. A non-relativistic free particle of mass m moving in one dimension has wavefunction

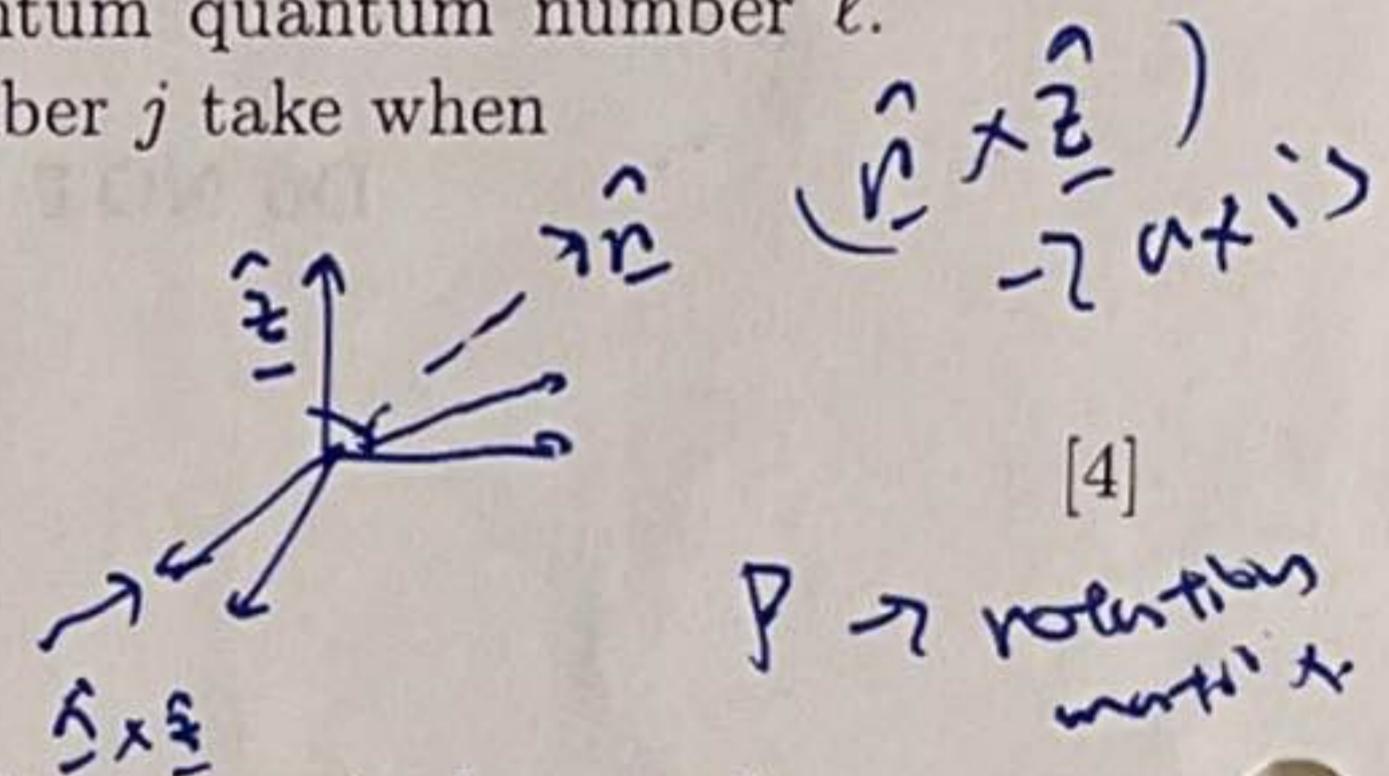
$$\psi(x, t) = A \exp\left(\frac{i}{\hbar}(px - E(p)t)\right) + A R \exp\left(-\frac{i}{\hbar}(px + E(p)t)\right),$$

where A and R are constants. Find $E(p)$. At time $t = 0$ the momentum of the particle is measured. What are the possible outcomes and their respective probabilities? [6]

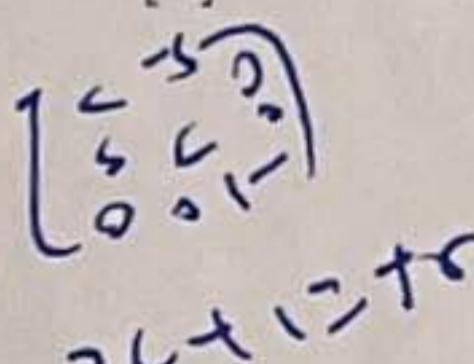
4. An electron is in a state with orbital angular momentum quantum number ℓ . What values may its total angular momentum quantum number j take when

(a) $\ell = 0$,

(b) $\ell = 1$?



5. Describe the *Zeeman Effect*. What magnetic flux density is required to produce a Zeeman splitting of 0.05 cm^{-1} in the ground state of hydrogen? [6]



6. Determine whether the following matrices represent a rotation in three dimensions and, if so, find the angle and axis of rotation:

$$(a) \frac{1}{\sqrt{6}} \begin{pmatrix} \sqrt{2} & 1 & \sqrt{3} \\ \sqrt{2} & 1 & -\sqrt{3} \\ \sqrt{2} & -2 & 0 \end{pmatrix}; \quad (b) \frac{1}{2} \begin{pmatrix} 1 + \frac{1}{\sqrt{2}} & 1 - \frac{1}{\sqrt{2}} & 1 \\ 1 - \frac{1}{\sqrt{2}} & 1 + \frac{1}{\sqrt{2}} & -1 \\ -1 & 1 & \sqrt{2} \end{pmatrix}.$$

[9]

Section B

7. Two non-interacting particles of the same mass m , and coordinates x_1 and x_2 respectively, occupy the same one-dimensional potential well $V(x)$. The energy eigenfunctions for a single particle in the well are denoted by $\phi_n(x)$, with $n = 1, 2, \dots$, and the corresponding energies, which are non-degenerate, by E_n . Write down the Hamiltonian for the two-particle system and show that

$$\Phi_{n_1, n_2}(x_1, x_2) = \phi_{n_1}(x_1)\phi_{n_2}(x_2)$$

are energy eigenfunctions. What is the corresponding energy eigenvalue? [4]

Explain briefly the meaning of *exchange symmetry*. [3]

In the following cases, state the degeneracy of the ground state and of the first excited state, and express the time-independent wavefunction for each of these states in terms of the functions $\Phi_{n_1, n_2}(x_1, x_2)$:

- (a) the particles are not identical and have spin zero;
- (b) the particles are identical and have spin zero.

Assume now that the particles are identical and have spin $\frac{1}{2}$. What are the possible spin states for the two particle system? What is the degeneracy of the ground state, and of the first excited state? Express the time-independent wavefunctions for all these states in terms of the functions $\Phi_{n_1, n_2}(x_1, x_2)$ and the spin states. [7]

8. Explain why a particle which is in an energy eigenstate cannot be moving in the classical sense. [3]

The simple harmonic oscillator has Hamiltonian H with eigenstates $|n\rangle$ and corresponding eigenvalues $E_n = \hbar\omega(n + \frac{1}{2})$, where $n = 0, 1, \dots$. At $t = 0$ the particle is in the state

$$|\Psi(t=0)\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle).$$

Show that at subsequent times the state of the particle is

$$|\Psi(t)\rangle = \frac{1}{\sqrt{2}}\left(e^{-iE_0t/\hbar}|0\rangle + e^{-iE_1t/\hbar}|1\rangle\right). \quad [5]$$

The time-independent wavefunctions for the ground and first excited states of the simple harmonic oscillator are

$$\phi_0(x) = \left(\frac{1}{a^2\pi}\right)^{\frac{1}{4}}e^{-x^2/2a^2} \quad \text{and} \quad \phi_1(x) = \left(\frac{4}{a^6\pi}\right)^{\frac{1}{4}}xe^{-x^2/2a^2},$$

$$e^{i\hat{H}t/\hbar}|4\rangle$$

where $a^2 = \hbar/m\omega$. Show that

$$\langle\Psi(t)|x|\Psi(t)\rangle = \frac{a}{\sqrt{2}}\cos(\omega t),$$

and calculate $\langle\Psi(t)|p|\Psi(t)\rangle$.

Find

$$\frac{d}{dt}\langle\Psi(t)|p|\Psi(t)\rangle + m\omega^2\langle\Psi(t)|x|\Psi(t)\rangle,$$

and comment on your result.

$$i\hbar\frac{\partial}{\partial x}|4\rangle = \hat{p}|4\rangle \quad [10]$$

$$i\hbar\frac{\partial}{\partial t}|4\rangle = \hat{H}|4\rangle dt$$

[2]

9. What is the physical origin of the *spin-orbit interaction*? For the electron in a hydrogen atom the spin-orbit contribution to the Hamiltonian is

$$H_{SO} = \frac{\mu_0}{4\pi} \frac{e^2}{2m_e^2} \frac{1}{r^3} \mathbf{l} \cdot \mathbf{s},$$

where r is the radial coordinate of the electron and \mathbf{l} and \mathbf{s} are the orbital and spin angular momentum operators respectively. Justify the form of this expression. (You are not required to explain the origin of $g_s = 2$ for the electron.) [10]

What is meant by the terms *conserved quantity* and *good quantum number*? [4]

Consider the electron in a hydrogen atom in the approximation that the Hamiltonian is given by

$$H = \frac{\mathbf{p}^2}{2m_e} - \frac{e^2}{4\pi\epsilon_0 r} + H_{SO}.$$

Is the z -component of orbital angular momentum a conserved quantity? You may assume that $[\mathbf{p}^2, l_z] = 0$. What is the implication of your result for the classification of the energy levels of the hydrogen atom? [6]

10. What is the purpose of *perturbation theory*?

[2]

A non-degenerate system has Hamiltonian H_0 whose eigenfunctions are $\phi_n(x)$, with corresponding eigenvalues E_n , where $n = 1, 2, \dots$. The Hamiltonian is modified by the addition of a term H_1 . Derive an expression for the first-order shift, ΔE_0 , in the energy of the ground state.

[8]

The one-dimensional infinite square well potential

$$\begin{aligned} V_0(x) &= 0, \quad 0 \leq x \leq a, \\ V_0(x) &= \infty, \quad \text{otherwise}, \end{aligned}$$

is modified by the addition of the perturbation

$$\begin{aligned} V_1(x) &= v, \quad 0 \leq x \leq \frac{a}{2}, \\ V_1(x) &= 0, \quad \text{otherwise}, \end{aligned}$$

where v is a constant. Show that all the energy levels of the system are shifted in first order by the same amount.

[6]

By considering the first-order shifted wavefunction ψ_n given by

$$\psi_n = \phi_n + \sum_{k \neq n} \frac{\langle \phi_k | V_1 | \phi_n \rangle}{E_n - E_k} \phi_k,$$

show that first-order perturbation theory is reliable, provided

$$v \ll \frac{3\hbar^2\pi^2}{2ma^2},$$

where m is the mass of the particle in the well.

$$\begin{aligned} \psi &= \phi^2 - \frac{1}{2} \\ \psi &\ll \frac{3\hbar^2\pi^2}{2ma^2} \\ v &\ll \frac{2\hbar^2\pi^2}{ma^2}. \end{aligned}$$

$$\begin{aligned} \psi_n(x) &= \sin\left(\frac{n\pi x}{a}\right) \\ (\phi_k | V_1 | \phi_n) &\ll E_n - E_k \\ \frac{1}{E_n} (E_n - E_k) &\ll \frac{1}{E_n} \end{aligned}$$

1. Classical theory predicts that if we increase the intensity of light incident on the metal plate, the emitted electrons will have more higher energy.

But in reality the ~~to~~ energy of electrons only depends (proportional) to the frequency of incident light.

Quantum Theory resolves this by stating that light ~~comes with~~ is composed of ~~with~~ quanta of energy called photons. Each photon has energy $\hbar\omega$ (ω is angular frequency $= 2\pi f$)

If energy of photon is not high ~~ever~~ enough then ~~electri~~ electrons will not be emitted

$$2 \quad S_x S_y = \left(\frac{\hbar}{2}\right)^2 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} = i \left(\frac{\hbar}{2}\right)^2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$S_y S_x = \left(\frac{\hbar}{2}\right)^2 \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = -\left(\frac{\hbar}{2}\right)^2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\rightarrow [S_x, S_y] = S_x S_y - S_y S_x = 2i \left(\frac{\hbar}{2}\right)^2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$= i\hbar \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = i\hbar S_z$$

$$\rightarrow [S_y, S_x] = -i\hbar \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = -i\hbar S_z$$

$$S_x S_z S_x = \left(\frac{\hbar}{2}\right)^2 \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

$$S_x S_z = -\left(\frac{\hbar}{2}\right)^2 \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

$$\rightarrow [S_x, S_z] = -i\hbar S_y$$

$$\rightarrow [S_z, S_x] = i\hbar S_y$$

$$S_y S_z = \left(\frac{\hbar}{2}\right)^2 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$S_z S_y = -\left(\frac{\hbar}{2}\right)^2 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\rightarrow [S_y, S_z] = i\hbar S_x$$

$$[S_z, S_y] = -i\hbar S_x$$

Hence S_x, S_y, S_z satisfy

$$[S_x, S_y] = i\hbar \epsilon_{ijk} S_k$$

→ Angular momentum.

Eigenvalues λ :

$$S_x |\psi\rangle = \lambda |\psi\rangle$$

$$\cancel{\det\left(\frac{\hbar}{2} \begin{pmatrix} 0-\lambda & 1 \\ 1 & 0+\lambda \end{pmatrix}\right) = 0}$$

$$\cancel{\lambda^2 - 1 = 0} \rightarrow \lambda = 1 \text{ or } -1$$

$$\lambda = 1 : \text{let } |\psi\rangle = \begin{pmatrix} a \\ b \end{pmatrix} \quad \text{let } + \cancel{\lambda} |\psi\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$$

$$\det \begin{pmatrix} 0-\lambda & \hbar/2 \\ \hbar/2 & 0-\lambda \end{pmatrix} = 0$$

$$\rightarrow \lambda^2 - (\frac{\hbar}{2})^2 = 0$$

$$\rightarrow \lambda = +\frac{\hbar}{2} \text{ or } -\frac{\hbar}{2}$$

If $\lambda = +\frac{\hbar}{2}$

$$\frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} a \\ b \end{pmatrix}$$

$$\rightarrow a=1 \rightarrow \text{normalize} \rightarrow |\psi\rangle = \frac{1}{\sqrt{2}} (1)$$

If $\lambda = -\frac{\hbar}{2}$

$$-\frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} a \\ b \end{pmatrix}$$

$$\rightarrow a=-b \rightarrow \text{normalize} \rightarrow |\psi\rangle = \frac{1}{\sqrt{2}} (-1)$$

$$3. \psi(x, t) = A \exp\left(\frac{i}{\hbar}(px - E(p)t)\right) + A \exp\left(-\frac{i}{\hbar}(px + E(p)t)\right)$$

ψ satisfies the Schrödinger equation

$$\rightarrow i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi$$

for free particle

$$\hat{H} = \frac{\hat{P}^2}{2m} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

$$i\hbar \frac{\partial \psi}{\partial t} = i\hbar A \left(-\frac{i}{\hbar}\right) E(p) \exp\left(\frac{i}{\hbar}(px - E(p)t)\right)$$

$$+ i\hbar A R \left(-\frac{i}{\hbar}\right) E(p) \exp\left(-\frac{i}{\hbar}(px + E(p)t)\right)$$

$$= \cancel{A} \cancel{(i\hbar R)} \exp\left(\frac{ipx}{\hbar}\right) \exp\left(-\frac{iE(p)t}{\hbar}\right) \times \cancel{E(p)}$$

$$= A E(p) \exp\left(\frac{i}{\hbar}(px - E(p)t)\right) + A R E(p) \exp\left(-\frac{i}{\hbar}(px + E(p)t)\right)$$

$$\hat{H}\psi = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} = \left(-\frac{\hbar^2}{2m}\right) \left(-\frac{1}{\hbar^2}\right) P^2 \text{ or } A \exp\left(\frac{i}{\hbar}(px - E(p)t)\right)$$

$$+ \left(-\frac{\hbar^2}{2m}\right) \left(-\frac{1}{\hbar^2}\right) (p)^2 A R \exp\left(-\frac{i}{\hbar}(px + E(p)t)\right)$$

$$= A \frac{P^2}{2m} \exp\left(\frac{i}{\hbar}(px - E(p)t)\right)$$

$$+ A R \frac{P^2}{2m} \exp\left(-\frac{i}{\hbar}(px + E(p)t)\right)$$

$$\rightarrow E(p) = \underbrace{\frac{P^2}{2m}}$$

At $t=0$

$$\psi(x, 0) = A \exp\left(\frac{ipx}{\hbar}\right) + A R \exp\left(-\frac{ipx}{\hbar}\right)$$

$\exp(\pm \frac{ipx}{\hbar})$ are eigenfunctions eigenvectors of the momentum operator $\hat{P} = -i\hbar \frac{\partial}{\partial x}$ with eigenvalues p and $-p$

\rightarrow possible outcomes $P, -P$

Probabilities

$$P(p) = \frac{1}{\sqrt{1+R^2}} \left[\frac{1}{1+R^2} \right]$$

$$P(-p) = \frac{R^2}{\sqrt{1+R^2}} \left[\frac{R^2}{1+R^2} \right]$$

4. (a) ~~so~~ electrons $\rightarrow S = \frac{1}{2}$

j goes from $|l-s|, |l-s|+1, \dots$ to $|l+s|$

$$\rightarrow \text{if } l=0, S = \frac{1}{2} \quad |l-s| = |l+s| = \frac{1}{2}$$

$$\rightarrow j = \frac{1}{2}$$

$$(b) \text{ if } l=1, S = \frac{1}{2}, |l-s| = \frac{1}{2}, l+s = \frac{3}{2}$$

$$\therefore j = \frac{1}{2} \text{ or } \frac{3}{2}$$

5.

Zeeman splitting : $E_{\pm} = E_0 \pm \mu_B B$ ($\mu_B = \frac{e\hbar}{2me}$)
of ground state hydrogen

$$\Delta E = |E_+ - E_-| = 2\mu_B B$$

$$\cancel{\nu = \frac{c}{\lambda}} \quad h\nu = \Delta E = 2\mu_B B$$

$$\omega = 2\pi f = \frac{2\pi c}{\lambda} \quad \therefore \bar{\nu} = \frac{1}{\lambda}$$

$$\therefore \omega = 2\pi c \bar{\nu}$$

$$\therefore \cancel{\nu} = 2\pi c \bar{\nu} \hbar = 2\mu_B B$$

$$\therefore h c \bar{\nu} = 2\mu_B B$$

$$\rightarrow B = \frac{h c \bar{\nu}}{2\mu_B} = \frac{2\pi c \bar{\nu} \cdot me}{2e\hbar}$$
$$= \frac{2\pi c \bar{\nu} me}{e}$$

$$V = 0.53 \text{ cm}^{-1} \text{ or } 5 \text{ m}^{-1}$$

$$= \cancel{0.0537} \quad \underline{0.054 \text{ T}}$$

6. (a)

$$A = \frac{1}{\sqrt{6}} \begin{pmatrix} \sqrt{2} & 1 & \sqrt{3} \\ \sqrt{2} & 1 & -\sqrt{3} \\ \sqrt{2} & -2 & 0 \end{pmatrix}$$

$$A^T A = I \quad \text{and} \quad \det(A) = 1$$

$$\begin{aligned} A^T A &= \frac{1}{6} \begin{pmatrix} \sqrt{2} & \sqrt{2} & \sqrt{2} \\ 1 & 1 & -2 \\ \sqrt{2} & -\sqrt{2} & 0 \end{pmatrix} \begin{pmatrix} \sqrt{2} & 1 & \sqrt{3} \\ \sqrt{2} & 1 & -\sqrt{3} \\ \sqrt{2} & -2 & 0 \end{pmatrix} \\ &= \frac{1}{6} \begin{pmatrix} 6 & 0 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 6 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = I \quad \checkmark \end{aligned}$$

$$\begin{aligned} \det(A) &= \left(\frac{1}{\sqrt{6}}\right)^3 [\sqrt{2}(0 - 2\sqrt{3}) - 1(0 + \sqrt{6}) + \sqrt{3}(-2\sqrt{2} - \sqrt{2})] \\ &= -1 \quad \times \end{aligned}$$

\rightarrow A is Not a rotation (but a rotation plus a reflection)

$$(b) B = \frac{1}{2} \begin{pmatrix} 1 + \frac{1}{2} & 1 - \frac{1}{2} & -1 \\ 1 - \frac{1}{2} & 1 + \frac{1}{2} & 1 \\ 1 & -1 & \sqrt{2} \end{pmatrix}$$

$$B^T B = \frac{1}{4} \begin{pmatrix} 1 + \frac{1}{2} & 1 - \frac{1}{2} & -1 \\ 1 - \frac{1}{2} & 1 + \frac{1}{2} & 1 \\ 1 & -1 & \sqrt{2} \end{pmatrix} \begin{pmatrix} 1 + \frac{1}{2} & 1 - \frac{1}{2} & 1 \\ 1 - \frac{1}{2} & 1 + \frac{1}{2} & -1 \\ -1 & 1 & \sqrt{2} \end{pmatrix}$$

$$= \frac{1}{4} \begin{pmatrix} 4 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{pmatrix} = I \quad \checkmark$$

$$\det(B) = \left(\frac{1}{2}\right)^3 [(1 + \frac{1}{2})(\sqrt{2}(1 + \frac{1}{2}) - (-1))]$$

$$- (1 - \frac{1}{2})((-1 - \frac{1}{2})\sqrt{2} - (1)) + (1)((-1 - \frac{1}{2}) + (1 + \frac{1}{2}))]$$

$$= 1 \quad \checkmark$$

$\rightarrow B$ is a rotation

Angle of rotation θ given by,

$$2\cos\theta + 1 = \text{tr}(B)$$

$$\rightarrow \cos\theta = \frac{\text{tr}(B) - 1}{2}$$

$$= \frac{\left[\frac{2+2\sqrt{2}}{2} \right] - 1}{2} = \frac{\sqrt{2}}{2}$$

$$\rightarrow \theta = \frac{\pi}{4} = 45^\circ$$

axis of rotation $\hat{n} = (a, b, c)^T$ is

$$B\hat{n} = \hat{n}$$

$$\rightarrow \frac{1}{2} \begin{pmatrix} 1+\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 1 \\ -\frac{1}{\sqrt{2}} & 1+\frac{1}{\sqrt{2}} & -1 \\ -1 & 1 & \sqrt{2}-2 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

$$\rightarrow \frac{1}{2} \begin{pmatrix} -1+\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 1 \\ -\frac{1}{\sqrt{2}} & -1+\frac{1}{\sqrt{2}} & -1 \\ -1 & 1 & \sqrt{2}-2 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$\rightarrow -a(1-\frac{1}{\sqrt{2}}) + b(1-\frac{1}{\sqrt{2}}) + c = 0 \quad ①$$

$$a(1-\frac{1}{\sqrt{2}}) - b(1-\frac{1}{\sqrt{2}}) - c = 0 \quad ②$$

$$-a + b + (\sqrt{2}-2)c = 0 \quad ③$$

~~① + ② = 2~~

$$① \times (2+\sqrt{2}) \Rightarrow -a + b + (2+\sqrt{2})c = 0 \quad ④$$

$$④ - ① \Rightarrow c = 0 \Rightarrow a = b.$$

$$\rightarrow \hat{n} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \text{ is the axis of rotation}$$

7. 2 non-interacting particles

$$\rightarrow \hat{H}_{12} = \hat{H}_1 + \hat{H}_2 + \underset{=0}{\underset{\downarrow}{\text{Hint}}} = \hat{H}_1 + \hat{H}_2$$

$$\begin{aligned}\rightarrow \hat{H}_{12} &= \frac{\hat{p}_1^2}{2m} + V(x_1) + \frac{\hat{p}_2^2}{2m} + V(x_2) \\ &= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2} + V(x_1) - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_2^2} + V(x_2)\end{aligned}$$

Substitute $\Phi_{n_1, n_2}(x_1, x_2)$ into TISE \Rightarrow

$$\begin{aligned}\hat{H}_{12} \Phi_{n_1, n_2}(x_1, x_2) &= \left(-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) + (V(x_1) + V(x_2)) \right) \Phi_{n_1, n_2}(x_1, x_2) \\ &= -\frac{\hbar^2}{2m} \phi_{n_2}(x_2) \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2} + V(x_1) \right] \phi_{n_1}(x_1) \\ &\quad + \phi_{n_1}(x_1) \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_2^2} + V(x_2) \right] \phi_{n_2}(x_2)\end{aligned}$$

\therefore operator of x_1 does nothing to function of only x_2 , and vice versa.

$$\begin{aligned}&= \phi_{n_2}(x_2) E_{n_1} \phi_{n_1}(x_1) + \phi_{n_1}(x_1) E_{n_2} \phi_{n_2}(x_2) \\ &= (E_{n_1} + E_{n_2}) \phi_{n_1}(x_1) \phi_{n_2}(x_2) \\ &= (E_{n_1} + E_{n_2}) \Phi_{n_1, n_2}(x_1, x_2)\end{aligned}$$

$\Rightarrow \Phi_{n_1, n_2}(x_1, x_2)$ are eigenfunctions with energy eigenvalues $E_{n_1} + E_{n_2}$

exchange symmetry applies for indistinguishable particles \rightarrow probability of observables shouldn't change if particles are exchanged.

$$|\Psi(x_1, x_2)|^2 = |\Psi(x_2, x_1)|^2$$

$$\rightarrow \underline{\Psi(x_2, x_1)} \quad \Psi(x_2, x_1) = e^{i\phi} \Psi(x_1, x_2)$$

If we exchange again :

~~Ψ~~ $\Psi(x_1, x_2) = e^{i\phi} \Psi(x_1, x_2)$

$$\rightarrow (e^{i\phi})^2 = 1 \rightarrow e^{i\phi} = \pm 1$$

$$\therefore \Psi(x_2, x_1) = \pm \Psi(x_1, x_2)$$

\rightarrow This is exchange symmetry. When

~~good~~ particles are exchanged the total wavefunction is unchanged or negative of the original wavefunction (~~function~~) \rightarrow (antisymmetric)

~~(fermions)~~ spin 0 so only consider spatial function.
particles ~~are~~ are bosons.

(a) not identical :

ground state: ~~Ψ~~ $\Psi(x_1, x_2) = \phi_1(x_1) \phi_1(x_2)$

degeneracy = 1

first excited states:

$$\Psi(x_1, x_2) = \phi_1(x_1) \phi_2(x_2)$$

$$\text{or } \phi_1(x_2) \phi_2(x_1)$$

degeneracy = 2

(b) identical :

ground state: $\Psi(x_1, x_2) = \phi_1(x_1) \phi_1(x_2)$

degeneracy = 1

first excited state: $\Psi(x_1, x_2) =$

$$= \frac{1}{\sqrt{2}} (\phi_1(x_1) \phi_2(x_2) + \phi_1(x_2) \phi_2(x_1))$$

degeneracy = 1

Identical particles, spin $-\frac{1}{2}$ Fermions:

possible spin states:

$$|\psi_s\rangle = |\uparrow_1\rangle |\uparrow_2\rangle$$

$$\text{or } \frac{1}{\sqrt{2}} (|\uparrow_1\rangle |\downarrow_2\rangle + |\downarrow_1\rangle |\uparrow_2\rangle) \quad \left. \right\} \text{symmetric}$$

$$\text{or } |\downarrow_1\rangle |\downarrow_2\rangle$$

$$\text{or } \frac{1}{\sqrt{2}} (|\uparrow_1\rangle |\downarrow_2\rangle - |\downarrow_1\rangle |\uparrow_2\rangle) \rightarrow \text{anti-symmetric}$$

Wavefunction of identical fermions is anti-symmetric, and consists of spatial wavefunction $\Psi = \Phi_{n,m}(x_1, x_2)$, and spin wavefunction $|\psi_s\rangle$

Ground state:

~~spatial function wave~~

$$\Psi = \phi_1(x_1) \phi_2(x_2) \text{ is symmetric}$$

$\Rightarrow |\psi_s\rangle$ must be anti-symmetric

\therefore Overall wavefunction

$$\underline{\Psi = \phi_1(x_1) \phi_2(x_2) \otimes \frac{1}{\sqrt{2}} (|\uparrow_1\rangle |\downarrow_2\rangle - |\downarrow_1\rangle |\uparrow_2\rangle)}$$

degeneracy = 1

First excited state:

If spin part is symmetric, then spatial part is anti-symmetric

$$\rightarrow \Psi = \frac{1}{\sqrt{2}} (\phi_1(x_1)\phi_2(x_2) - \phi_1(x_2)\phi_2(x_1))$$

$$|\Psi_s\rangle = |\uparrow_1\rangle|\uparrow_2\rangle$$

$$\text{or } \frac{1}{\sqrt{2}} (|\uparrow_1\rangle|\downarrow_2\rangle + |\downarrow_1\rangle|\uparrow_2\rangle)$$

$$\text{or } |\downarrow_1\rangle|\downarrow_2\rangle$$

$$\Psi = \Psi \otimes |\Psi_s\rangle$$

if spin part is ~~not~~ anti-symmetric, then
spatial part is symmetric

$$\Psi = \frac{1}{\sqrt{2}} (\phi_1(x_1)\phi_2(x_2) + \phi_1(x_2)\phi_2(x_1))$$

$$\otimes \frac{1}{\sqrt{2}} (|\uparrow_1\rangle|\downarrow_2\rangle - |\downarrow_1\rangle|\uparrow_2\rangle)$$

$$\rightarrow \text{degeneracy} = 4$$

8. If a particle is in an energy eigenstate, then $|E_n\rangle$, then the time evolution of this state is given by $\langle E_n(t) \rangle = |E_n\rangle \exp(-iE_n t/\hbar)$

If the spatial wavefunction ~~$\psi_{E_n}(x)$~~

$$\begin{aligned}\psi_{E_n}(x,t) &= \langle x | E_n(t) \rangle = \langle x | E_n \rangle e^{-\frac{iE_n t}{\hbar}} \\ &= \psi_{E_n}(x,0) e^{-\frac{iE_n t}{\hbar}}\end{aligned}$$

The probability of finding the particle in position between $[x, x+dx]$ is

$$\begin{aligned}|\psi_{E_n}(x,t)|^2 &= |\psi_{E_n}(x,0)|^2 e^{\frac{iE_n t}{\hbar}} e^{-\frac{iE_n t}{\hbar}} \\ &= |\psi_{E_n}(x,0)|^2 \rightarrow \text{time independent.}\end{aligned}$$

\therefore The probability density of particle being found anywhere in space is constant in time

\rightarrow particle is not moving classically.

$$\text{TDSE : } i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = \hat{H} |\psi(t)\rangle$$

$\because |0\rangle, |1\rangle, \dots |n\rangle, \dots$ are eigenstates

$$\therefore \hat{H} |n\rangle = E_n |n\rangle$$

$$\text{try } |\psi(t)\rangle = \frac{1}{\sqrt{2}} (e^{-iE_0 t/\hbar} |0\rangle + e^{-iE_1 t/\hbar} |1\rangle)$$

into TDSE :

$$\begin{aligned}i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} &= i\hbar \left(\frac{1}{\sqrt{2}}\right) \left(-\frac{i}{\hbar} (E_0 e^{-iE_0 t/\hbar} |0\rangle + E_1 e^{-iE_1 t/\hbar} |1\rangle)\right) \\ &= \frac{1}{\sqrt{2}} (E_0 e^{-iE_0 t/\hbar} |0\rangle + E_1 e^{-iE_1 t/\hbar} |1\rangle)\end{aligned}$$

$$\begin{aligned}\hat{H} |\psi(t)\rangle &= \frac{1}{\hbar} (e^{-iE_0 t/\hbar} \hat{H} |0\rangle + e^{-iE_1 t/\hbar} \hat{H} |1\rangle) \\ &= \frac{1}{\sqrt{2}} (E_0 e^{-iE_0 t/\hbar} |0\rangle + E_1 e^{-iE_1 t/\hbar} |1\rangle)\end{aligned}$$

$$\rightarrow i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \text{ satisfied } \checkmark$$

i.e. sub $t=0$ into $|\psi(t)\rangle$ we get

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \text{ consistent } \checkmark$$

$|\psi(t)\rangle$ is the state of the particle.

$$\langle x|\psi(t)\rangle = \frac{1}{\sqrt{2}} (e^{-iE_0 t/\hbar}$$

$$\langle 4(t)|x|\psi(t)\rangle = \frac{1}{2} (\langle 0|x|0\rangle + \langle 1|x|1\rangle$$

$$+ e^{-i(E_1 - E_0)t/\hbar} \langle 0|x|1\rangle$$

$$+ e^{i(E_1 - E_0)t/\hbar} \langle 1|x|0\rangle)$$

$$= \frac{1}{2} (\langle 0|x|0\rangle + \langle 1|x|1\rangle + 2 \operatorname{Re}[e^{i(E_1 - E_0)t/\hbar} \langle 1|x|0\rangle])$$

$$\langle 0|x|0\rangle = \int_{-\infty}^{\infty} dx \times \phi_0^2 = 0$$

\uparrow
odd \uparrow
even

$$\langle 1|x|1\rangle = \int_{-\infty}^{\infty} dx \cdot x \cdot \phi_1^2 = 0$$

\uparrow
odd \uparrow
even

$$\langle 1|x|0\rangle = \int_{-\infty}^{\infty} dx \cdot x \cdot \phi_0 \phi_1$$

$$= \left(\frac{4}{a^8 \pi^2} \right)^{\frac{1}{4}} \int_{-\infty}^{\infty} dx \cdot x^2 e^{-x^2/a^2}$$

$\underbrace{\quad}_{\frac{\sqrt{\pi}}{2} a^3}$

$$= \frac{\sqrt{2}}{a^2 \sqrt{\pi}} \cdot \frac{\sqrt{\pi}}{2} a^3 = \frac{\sqrt{2}}{2} a = \frac{a}{\sqrt{2}}$$

$$\rightarrow \langle \psi(t) | \times | \psi(t) \rangle$$

$$= \frac{1}{2} \cdot 2 \cdot \frac{\alpha}{\hbar} \operatorname{Re} [e^{i(E_1 - E_0)t/\hbar}]$$

$$= \frac{\alpha}{\hbar} \cos \left(\frac{E_1 - E_0}{\hbar} t \right)$$

$$= \frac{\alpha}{\hbar} \cos(\omega t)$$

$$P = -i\hbar \frac{\partial}{\partial x}$$

$$\langle \psi(t) | P | \psi(t) \rangle = \frac{1}{2} (\langle 0|P|0\rangle + \langle 1|P|1\rangle) + 2\operatorname{Re} [e^{i(E_1 - E_0)t/\hbar} \langle 1|P|0\rangle]$$

$$\langle 0|P|0\rangle \propto \int dx e^{-x^2/a^2} \frac{\partial}{\partial x} (e^{-x^2/a^2}) = 0$$

↓
gives even x

even x odd

$$\begin{aligned} \langle 1|P|1\rangle &\propto \int dx x e^{-x^2/a^2} \frac{\partial}{\partial x} (x e^{-x^2/a^2}) \\ &\propto \int dx x (e^{-x^2/a^2}) (e^{-x^2/a^2} + x^2 e^{-x^2/a^2}) \\ &\propto \int dx (\text{odd} + \text{odd}) \\ &= 0 \end{aligned}$$

$$\langle 1|P|0\rangle = -i\hbar \frac{\partial}{\partial x} \langle 0| \int_{-\infty}^{\infty} dx \phi_1 \left(\frac{\partial}{\partial x} \phi_0 \right)$$

$$= -i\hbar \left(\frac{4}{a^8 \pi^2} \right)^{\frac{1}{4}} \int_{-\infty}^{\infty} (x e^{-x^2/a^2}) \frac{\partial}{\partial x} (e^{-x^2/a^2})$$

$$= -i\hbar \left(\frac{4}{a^8 \pi^2} \right)^{\frac{1}{4}} \int_{-\infty}^{\infty} \left(-\frac{1}{a^2} \right) dx x^2 e^{-x^2/a^2}$$

$$= i\hbar \frac{1}{a^2} \left(\frac{4}{a^8 \pi^2} \right)^{\frac{1}{4}} \int_{-\infty}^{\infty} dx x^2 e^{-x^2/a^2}$$

$$= \frac{1}{2} i\hbar \frac{1}{a^2} \left(\frac{4}{a^8 \pi^2} \right)^{\frac{1}{4}} \cdot \frac{\sqrt{\pi}}{2} a^3$$

$$= i\hbar \frac{a}{\sqrt{2}} \cdot \frac{1}{a^2} = \frac{i\hbar}{a\sqrt{2}}$$

$$\rightarrow \langle \psi(t) | P | \psi(t) \rangle = \operatorname{Re} \left[\frac{i\hbar}{a\sqrt{2}} e^{+i(E_1 - E_0)t/\hbar} \right]$$

$$= \frac{i\hbar}{a\sqrt{2}} \operatorname{Im} (e^{i(E_1 - E_0)t/\hbar})$$

$$= -\frac{\hbar}{a\sqrt{2}} \sin(\omega t)$$

$$\frac{d}{dt} \langle \psi(t) | P | \psi(t) \rangle = -\frac{\hbar\omega}{a\sqrt{2}} \cos(\omega t)$$

$$-\frac{\hbar\omega}{a\sqrt{2}} = -\frac{\hbar\omega^2 a}{a^2 \sqrt{2}} = -\underbrace{\frac{\hbar\omega \cdot m\omega \cdot a}{\sqrt{2}}}_{a^2 = \frac{\hbar}{m\omega}} = -m\omega^2 \frac{a}{\sqrt{2}}$$

$$\therefore \frac{d}{dt} \langle \psi(t) | P | \psi(t) \rangle + m\omega^2 \langle \psi(t) | x | \psi(t) \rangle$$

$$= -m\omega^2 \frac{a}{\sqrt{2}} \cos(\omega t) + m\omega^2 \frac{a}{\sqrt{2}} \cos(\omega t)$$

$$= 0$$

Classically the restoring force of SHO

$$\text{is } F = -m\omega^2 x \quad \therefore F = \frac{dp}{dt}$$

$$\therefore \frac{dp}{dt} = -m\omega^2 x \rightarrow \frac{dp}{dt} + m\omega^2 x = 0$$

replacing ~~the $\langle \psi | P | \psi \rangle$~~ $P \cdot x$ with $\langle \psi | P | \psi \rangle$, $\langle \psi | x | \psi \rangle$

gives the quantum version of this momentum-force relationship. $\left(\frac{d\langle p \rangle}{dt} = -\langle \frac{dx}{dt} \rangle \right)$

9.

→ Imagine the electron in orbit around the nucleus. From the electron's point of view, the proton is circling around it. This orbiting positive charge sets up a magnetic field \underline{B} in the electron frame, which exerts a torque on the spinning electron, tending to align its magnetic moment (\underline{m}) along the direction of the field.

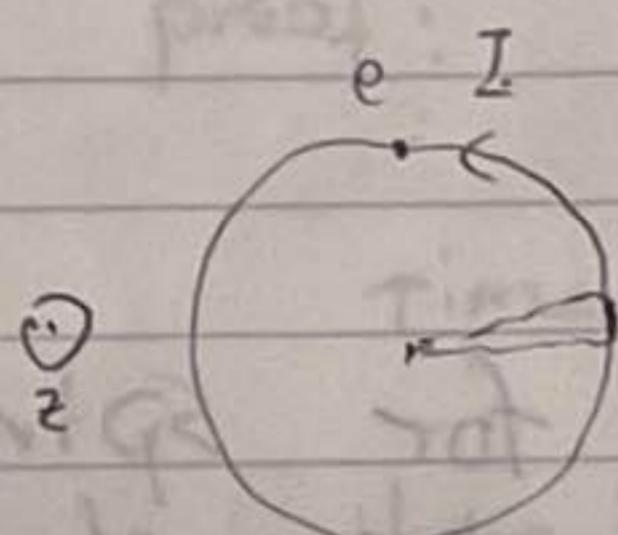
Eg Ignoring for now that this "electron frame" is not inertial.

The Hamiltonian (classical energy) of a magnetic dipole in a uniform \underline{B} -field is

$$H = - \underline{m} \cdot \underline{B}$$

- picture the proton as a continuous current loop

effective current $I = \frac{e}{T}$ ✓ charge of proton
= +e.



Biot-Savart Law

$$d\underline{B} = \frac{\mu_0}{4\pi} \frac{I d\underline{l} \times \hat{r}}{r^3} \quad \leftarrow d\underline{l} = r d\theta \text{ proton}$$

$$\underline{B} = \int d\underline{B} = \frac{\mu_0 I}{4\pi} \frac{r^2}{r^3} \int_0^{2\pi} d\theta = \frac{\mu_0 I}{2r}$$

$$\therefore \underline{B} = \frac{\mu_0 I}{2r} \hat{z} = \cancel{\frac{\mu_0}{4\pi}} \frac{\mu_0 e}{2r T} \frac{\frac{N_o e}{T} \hat{z}}{2r T}$$

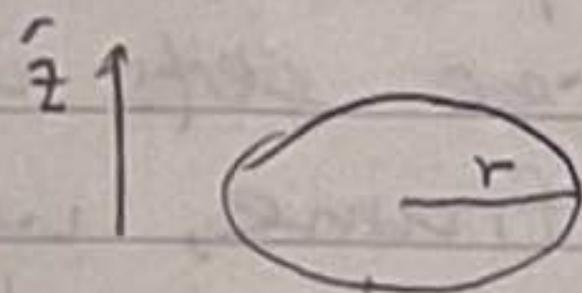
Orbital Angular momentum $\underline{L} = m v r \hat{z}$ $m r \times v = m v r \hat{z}$
 $= m_e \left(\frac{2\pi r}{T} \right) r \hat{z}$

\underline{B} and \underline{L} both along \hat{z} , so we can & take their ratio

$$\frac{B}{L} = \cancel{\frac{\mu_0 e}{2r T \cdot m_e^2 \pi r^2}} \frac{\frac{\mu_0 e \cdot T}{2r T \cdot m_e^2 \pi r^2}}{1} = \frac{\mu_0}{4\pi} \frac{e}{m_e} \frac{1}{r^3}$$

$$\rightarrow \underline{B} = \frac{\mu_0}{4\pi} \frac{e}{m_e r^3} \underline{L}$$

Now model the electron itself as a ring of charge spinning around its centre



$$I = mer^2$$

$$\underline{N} = \hat{z} (\text{current} \times \text{Area}) = \hat{z} \left(\frac{q}{T} \right) (\pi r^2) = \frac{2\pi r^2}{T} \hat{z}$$

$$\text{spin angular momentum } \underline{S} = \hat{z} I w \quad \begin{matrix} \text{angular} \\ \text{speed} \end{matrix}$$

momentum of inertia

$$\underline{S} = \hat{z} (mer^2) \left(\frac{2\pi}{T} \right)$$

$$\underline{N} \cdot \underline{S} \text{ both along } \hat{z} \rightarrow \frac{\underline{N}}{\underline{S}} = \frac{q\pi r^2 \cdot T}{T \cdot mer^2 \cdot 2\pi} = \frac{q}{2me}$$

$$\therefore \underline{\mu} = \frac{q}{2me} \underline{S}$$

(ignore the gyromagnetic ratio for spin)

$$\because q = -e \quad \therefore \underline{\mu} = -\frac{e}{2me} \underline{S}$$

$$\therefore H_{so} = -\underline{\mu} \cdot \underline{B}$$

$$= - \left(-\frac{e}{2me} \underline{S} \right) \cdot \left(\frac{\mu_0}{4\pi} \frac{e}{mer^3} \right) \underline{L}$$

$$\rightarrow H_{so} = \underbrace{\frac{\mu_0}{4\pi} \frac{e^2}{2me^2} \frac{1}{r^3} \underline{S} \cdot \underline{L}}_{\therefore [\hat{S}_i, \hat{L}_j] = 0}$$

$$\therefore H_{so} = \underbrace{\frac{\mu_0}{4\pi} \frac{e^2}{2me^2} \frac{1}{r^3} \underline{L} \cdot \underline{S}}$$

A conserved quantity is a quantity such that the expectation value of this quantity is time independent

$$\rightarrow \frac{d\langle Q \rangle}{dt} = \frac{1}{i\hbar} \langle [Q, H] \rangle = 0$$

$$\rightarrow [Q, H] = 0$$

conserved quantity commutes with the Hamiltonian.

A good quantum number is the eigenvalue of an eigenstate of an operator, such that this eigenstate remains ~~in the~~ an eigenstate of the operator as time evolves.

$$Q|q_i\rangle = q_i |q_i\rangle \text{ if } [Q, H] = 0$$

$$\langle Q|q_i(0)\rangle = q_i \langle q_i(0) \rangle$$

proof: Assume $[Q, H] = 0$ and $\hat{Q}|q_i\rangle = q_i |q_i\rangle$

time evolution operator $\hat{T}(t) = e^{\frac{-it\hat{H}}{\hbar}}$

$$\text{then } \hat{Q}|q_i(t)\rangle = \hat{Q}\hat{T}|q_i(0)\rangle = \hat{Q}e^{-\frac{it\hat{H}}{\hbar}}|q_i(0)\rangle$$

$$\text{if } [Q, H] = 0, \text{ then } [\hat{Q}, e^{it\hat{H}/\hbar}] = 0$$

$$\rightarrow \hat{Q}|q_i(t)\rangle = \hat{Q}e^{\frac{it\hat{H}}{\hbar}}\hat{Q}|q_i(0)\rangle = q_i e^{it\hat{H}/\hbar} |q_i(0)\rangle$$

$$= q_i |q_i(t)\rangle$$

of §

$|q_i(t)\rangle$ remains to be an eigenstate with the same eigenvalue q_i as $|q_i(0)\rangle$

\rightarrow A good quantum number is the eigenvalue of an operator that commutes with the Hamiltonian.

$$\text{If } \hat{H} = \frac{\hat{p}^2}{2me} - \frac{e^2}{4\pi\epsilon_0 r} + \hat{H}_{so}$$

$$= \frac{\hat{p}^2}{2me} - \frac{e^2}{4\pi\epsilon_0 r} + \frac{\mu_0 e^2}{4\pi 2me^2} \frac{1}{r^3} \hat{L} \cdot \hat{S}$$

$$\text{then consider } \hat{E}_z [\hat{L}_z, \hat{H}] = C_1 [\hat{L}_z, \hat{P}^2] + C_2 [\hat{L}_z, \frac{1}{r}] + C_3 [\hat{L}_z, \frac{1}{r^3} \hat{L} \cdot \hat{S}]$$

(C_1, C_2, C_3 are constants)

$$\text{ie } [\hat{L}_z, \hat{P}^2] = 0 \quad (\text{given})$$

$$[\hat{L}_z, \frac{1}{r}] = 0$$

↑
only operating
on θ, ϕ

↑
function only
of r

$$\cancel{\hat{L}_z + \frac{1}{r^3} \hat{L} \cdot \hat{S}} [\hat{L}_z, \frac{1}{r^3} \hat{L} \cdot \hat{S}] \propto [\hat{L}_z, \hat{L} \cdot \hat{S}]$$

↑
function only of r

$$\rightarrow \cancel{\hat{E}_z} [\hat{L}_z, \hat{H}] = C_4 [\hat{L}_z, \hat{L} \cdot \hat{S}]$$

$$[\hat{L}_z, \hat{L} \cdot \hat{S}] = [\hat{L}_z, L_x S_x + L_y S_y + L_z S_z]$$

$$= [\hat{L}_z, L_x] \hat{S}_x + L_x [\hat{L}_z, \hat{S}_x] + [\hat{L}_z, L_y] \hat{S}_y + L_y [\hat{L}_z, \hat{S}_y] \xrightarrow{\dots} = 0 \quad \because [L_i, S_j] = 0$$

$$+ [\hat{L}_z, L_z] \hat{S}_z + L_z [\hat{L}_z, \hat{S}_z] \\ \xrightarrow{\dots} = 0$$

$$= [\hat{L}_z, L_x] \hat{S}_x + [\hat{L}_z, L_y] \hat{S}_y$$

$$= i\hbar (L_y S_x - L_x S_y)$$

$$= \cancel{i\hbar} \cancel{L_z} i\hbar (\hat{S} \times \hat{L})_z \neq 0$$

$\therefore [\hat{L}_z, \hat{H}] \neq 0 \quad \therefore L_z \text{ is not conserved.}$

Consider $\hat{J} = \hat{L} + \hat{S}$ the total angular momentum

~~\hat{J}^2~~ we can check that $\cancel{[\hat{J}, \hat{L} \cdot \hat{S}]} = 0$ and

$\hat{J}^2, \hat{L}^2, \hat{S}^2$ all commute with \hat{H} . So we can use the eigenvalues of $\hat{J}^2, \hat{J}_z, \hat{L}^2, \hat{S}^2$, namely j, m_j, l, s (good quantum numbers) to represent a state $|j, j_m, l, s\rangle$

(We cannot use m_L , the eigenvalue of \hat{L}_z)

10. ~~where~~ ~~for~~ Perturbation theory enables us to approximate the solutions to the Schrödinger's equation ~~for~~ when the deviation of the actual Hamiltonian from ~~the~~ Hamiltonian that we already know the solution is small. We can use it to estimate the solutions to problems that cannot be solved exactly.

$$\hat{H} = \hat{H}_0 + \hat{H}_1 \quad \text{let } \hat{H}_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$$

~~Consider~~ ~~\hat{H}~~ ~~$= \hat{H}_0 + \hat{H}_1$~~

$$\text{let } \psi_i = \phi_i^{(0)} + \sum_{m=1}^{\infty} C_m \phi_m^{(0)}$$

$$\text{and } E_i = E_i^{(0)} + \Delta E_0$$

$$\text{then } \hat{H} \psi_i = E_i \psi_i, \quad \text{let } \psi_i = \phi_i^{(0)} + \sum_{m=1}^{\infty} C_m \phi_m^{(0)}$$

$$\Rightarrow (\hat{H}_0 + \hat{H}_1) (\phi_i^{(0)} + \sum_{m=1}^{\infty} C_m \phi_m^{(0)}) = (E_i^{(0)} + \Delta E_0) (\phi_i^{(0)} + \sum_{m=1}^{\infty} C_m \phi_m^{(0)})$$

$$\rightarrow (\hat{H}_0 + \hat{H}_1) (\phi_i^{(0)} + \sum_{m=1}^{\infty} C_m \phi_m^{(0)}) = (E_i^{(0)} + \Delta E_0) (\phi_i^{(0)} + \sum_{m=1}^{\infty} C_m \phi_m^{(0)})$$

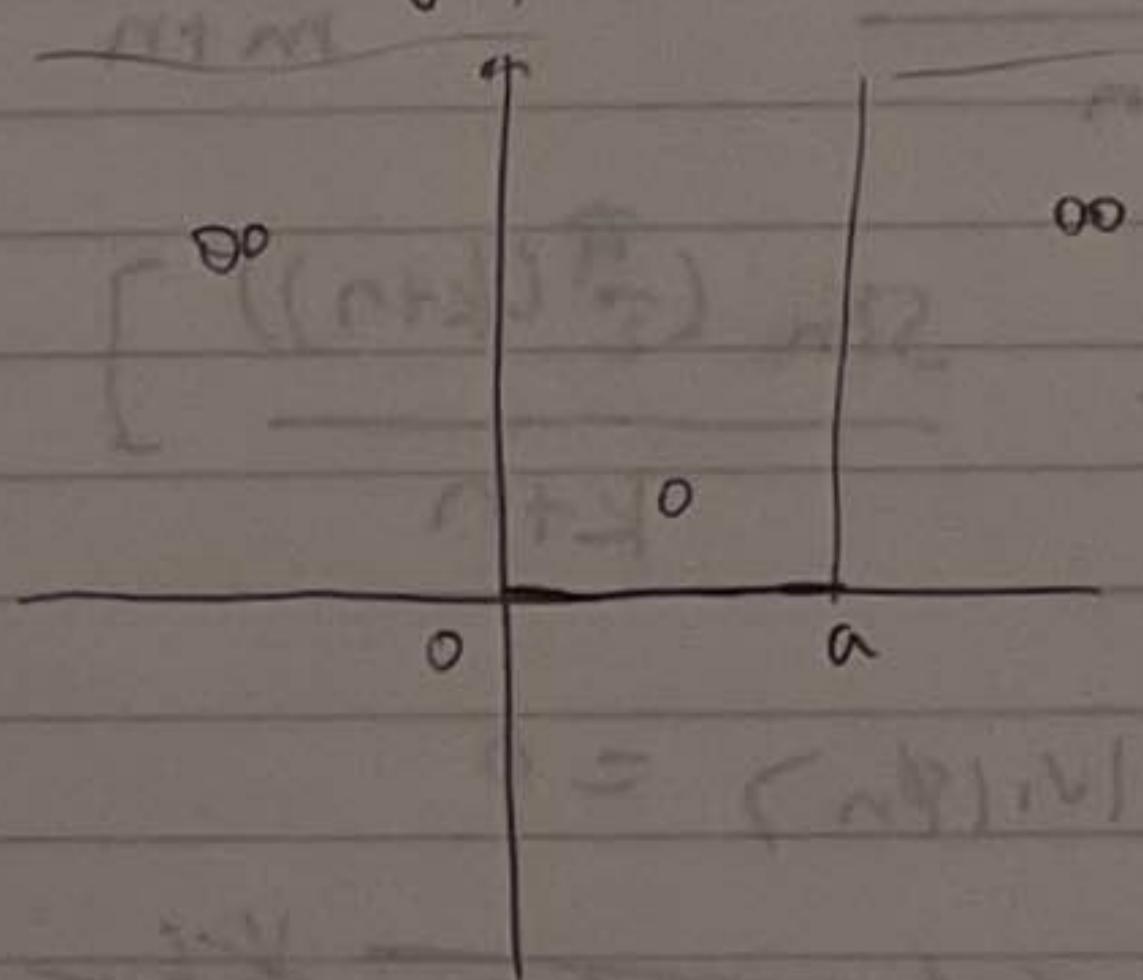
$$\Rightarrow \cancel{\hat{H}_0} \phi_i^{(0)} + \sum_{m=1}^{\infty} C_m \hat{H}_0 \phi_m^{(0)} + \hat{H}_1 \phi_i^{(0)} + \sum_{m=1}^{\infty} C_m \hat{H}_1 \phi_m^{(0)}$$

$$= E_i^{(0)} \phi_i^{(0)} + E_i^{(0)} \sum_{m=1}^{\infty} C_m \phi_m^{(0)} + \Delta E_0 \phi_i^{(0)} + \Delta E_0 \sum_{m=1}^{\infty} C_m \phi_m^{(0)} \quad (1)$$

\because all $\phi_m^{(0)}$'s are orthonormal

$$\therefore \cancel{\int dx \phi_i^{(0)} \int dx \psi_i^{(0)} (1)} \Rightarrow 0 \int dx \phi_i^{(0)} \hat{H}_1 \phi_i^{(0)} = \Delta E_0 \int dx \phi_i^{(0)} \phi_i^{(0)}$$

$$\rightarrow \Delta E_0 = \underbrace{\int dx \phi_i^{(0)} \hat{H}_1 \phi_i^{(0)}}_{\text{V(x)}}$$



For this infinite potential well

$$\phi_n^{(0)}(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \quad (0 \leq x \leq a)$$

$$\phi_n^{(0)} = 0 \quad \text{otherwise.}$$

$$E_n^{(0)} = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$

P perturbation

$$H_1 = \begin{cases} V & 0 \leq x \leq \frac{a}{2} \\ 0 & \text{otherwise} \end{cases}$$

First order shift in energy

$$\Delta E_n^{(1)} = \langle \phi_n^{(0)} | H_1 | \phi_n^{(0)} \rangle$$

$$= \int_{-\infty}^{\infty} dx |\phi_n^{(0)}|^2 H_1 = \cancel{\int_{-\infty}^{\infty}}$$

$$= \cancel{\int_0^a} = \frac{2V}{a} \int_0^{a/2} dx \sin^2\left(\frac{n\pi x}{a}\right)$$

$$= \left[\frac{x}{2} - \frac{a \sin\left(\frac{2\pi n x}{a}\right)}{4\pi n} \right]_0^{a/2} \times \frac{2V}{a}$$

$$= \frac{a}{4} \times \frac{2V}{a} = \frac{V}{2} \quad \text{independent of } n$$

\rightarrow All energy levels are shifted by the same amount

$$\psi_n(x) = \phi_n + \sum_{k \neq n} \frac{\langle \phi_k | V_1 | \phi_n \rangle}{E_n - E_k} \phi_k$$

$$\langle \phi_k | V_1 | \phi_n \rangle = \frac{2V}{a} \int_0^{a/2} \sin\left(\frac{n\pi x}{a}\right) \sin\left(\frac{k\pi x}{a}\right)$$

$$= \frac{2V}{a} \cdot \frac{a}{2\pi} \left[\frac{\sin\left(\frac{\pi x(k-n)}{a}\right)}{k-n} - \frac{\sin\left(\frac{\pi x(k+n)}{a}\right)}{m+n} \right]_0^{\frac{a}{2}}$$

$$= \frac{V}{\pi} \left[\frac{\sin\left(\frac{\pi}{2}(k-n)\right)}{k-n} - \frac{\sin\left(\frac{\pi}{2}(k+n)\right)}{k+n} \right]$$

\therefore if $k-n$ is even $\langle \phi_k | V_1 | \phi_n \rangle = 0$

If $k-n$ is odd. $\langle \phi_k | V_1 | \phi_n \rangle = \cancel{\frac{V}{\pi}}$

$$\rightarrow \langle \phi_k | V_1 | \phi_n \rangle = (-1)^{\frac{k-n-1}{2}} \frac{V}{\pi} \left[\frac{1}{k-n} - \frac{1}{k+n} \right]$$

$$= (-1)^{\frac{k-n-1}{2}} \frac{V}{\pi} \left[\frac{2n}{k^2 - n^2} \right]$$

$\therefore \langle \phi_k | V_1 | \phi_n \rangle$ is on the order of V
for perturbation theory to apply.

$$|\langle \phi_k | V_1 | \phi_n \rangle| \ll |E_n - E_k| \rightarrow V \ll |E_n - E_k|$$

The smallest $|E_n - E_k|$ is when $k=1, n=2$,
this gives $|E_n - E_k| = |n^2 - k^2| \frac{\pi^2 \hbar^2}{2ma^2} = (2^2 - 1^2) \frac{\pi^2 \hbar^2}{2ma^2}$

$$= \frac{3\hbar^2 \pi^2}{2ma^2}$$

$$\rightarrow V \ll \frac{3\hbar^2 \pi^2}{2ma^2}$$