I. Introduction

A. Black Body

- Empirical measurement
- High frequency: Wien's Law

$$u(\nu, T) = \nu^3 e^{\,-\beta\nu/T}$$

- Low frequency: Rayleigh-Jeans Law

$$u(\nu, T) = \frac{8\pi\nu^2}{c^3} kT$$

  - ◇ Diverges at high ν
- Plank: Interpolated the two fomulae and found

$$u(\nu, T) = \frac{8\pi h}{c^3} \frac{\nu^3}{\mathrm{e}^{h\nu/kT} - 1}$$

  - ◇ No understanding of its origin classically
  - ◇ Needed to assume $\varepsilon_n = nh\nu$ and apply Stat. Mech
- Quantum approach:
  - ◇ Bose-Einstein Statistics

$$\bar{n} = \frac{1}{\mathrm{e}^{\beta\varepsilon} - 1}$$

  - ◇ Density of states

$$\begin{aligned} g(k)dk &= \frac{2L^3}{(2\pi)^3} d^3k = \frac{2(4\pi)k^2 dk}{(2\pi)^3} = g(\nu)d\nu \\ g(\nu) &= \frac{8\pi\nu^2}{c^3} \end{aligned}$$

  - ◇ Energy density:

$$\begin{aligned} u(\nu, T) &= g(\nu)\bar{n}(\nu)\varepsilon \\ &= \frac{8\pi\nu^2}{c^3} \frac{h\nu}{\mathrm{e}^{h\nu/kT} - 1} \end{aligned}$$

B. Photoelectric Effect

- $\frac{1}{2}mv^2 = h\nu - W = eV_r$
- $W \equiv$ potential threshold

- $\diamond$ Higher intensity $\Rightarrow$ More photons $\Rightarrow$ More e$^-$
- $\diamond$ Higher energy $\Rightarrow$ Higher energy e$^-$

- Could eliminate the current simply by raising V_r high enough
- Strong evidence that light was traveling in packets of energy

C. Bohr Atom

- Observed Hydrogen spectral lines with spacing $E \propto 1/n^2$
- Postulated the electron has quantized angular momenta (stationary states)

$$\ell = n\hbar = mvr$$

- Bohr radii (balance forces)

$$\begin{aligned} \frac{e^2}{r^2} &= \frac{mv^2}{r} \\ \Rightarrow\ r &= \frac{n^2\hbar^2}{e^2 m} \end{aligned}$$

- Energy:

$$\begin{aligned} E &= \frac{1}{2}mv^2 - \frac{e^2}{r} \\ &= -\frac{e^4 m}{2\hbar^2 n^2} \end{aligned}$$

- Bohr introduced
  (a) Correspondence Principle
  (b) Quantized Angular Momentum

D. Compton Effect

- Most compelling evidence of photons
- $p = h\nu/c$
- $\lambda' - \lambda = \frac{h}{mc}(1 - \cos\theta)$
- Compton wavelength of e$^-$: $h/mc = 2.4 \times 10^{-10}$ cm

E. Electron Diffraction

- De Broglie – Theoretical prediction: $\lambda = h/p$
- Experiment – e$^-$ Interference: $\lambda = 2a\sin\theta/n$

II. Wave Mechanics

A. Motivation

- Inspired by wave-particle duality
- Light
  - ◇ Governed by Maxwell's equations

$$\nabla^2 \vec{E} - \frac{1}{c^2}\frac{\partial^2 \vec{E}}{\partial t^2} = 0 \tag{1}$$

  - ◇ $E(r,t), B(r,t)$ fields are physical
  - ◇ Photons: Directed by an EM wave with plane wave solution:

$$\vec{E} = E_0 \hat{x} \ \cos\left[\, k(z \pm ct) \,\right] \tag{2}$$

- Particles?
  - ◇ Goal: Devise a wave function analogous to $E(r,t)$ and a set of equations analogous to Maxwell's equations
  - ◇ Result: Wave function
    - ▲ Non-physical (not directly measurable)
    - ▲ No equations analogous to Maxwell
    - ▲ And (by the way) **none of this can be derived!!!**

B. Wave Function

- Free particle with momentum p
  - ◇ Debroigle: Consider a wavelength $\lambda = h/p$ or

$$k = \frac{2\pi}{\lambda} = p/\hbar$$

- Plane Wave
  - ◇ Standard equation

$$\Psi(x,t) = A\mathrm{e}^{i(kx-\omega t)} \tag{3}$$

  - ◇ with

$$\omega = \omega(k)$$

- Phase velocity: $v_p = \omega/k$
- Amplitude: $|\Psi|^2 = |A|^2$ independent of x, t
  - ◇ Where is the particle?
  - ◇ Even the real part of Ψ has wiggles

C. Building a particle

- Goal: Localize at $x = 0$ at $t = 0$ with $p_0 = \hbar k_0$
- Positively interfere many plane waves with varying λ

$$\Psi(x, t = 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k)\, \mathrm{e}^{ikx} dk \tag{4}$$

  - ◇ Inverting, we find (standard Fourier analysis)

$$A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x, t = 0)\, \mathrm{e}^{-ikx} dx \tag{5}$$

- Each wave propagates in time as $\mathrm{e}^{-i\omega t}$

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k)\, \mathrm{e}^{i(kx - \omega t)} dk \tag{6}$$

- To give the particle a momentum, require $A(k)$ is peaked at k_0 with width $\Delta k \ll k_0$
- At time t we want an appreciable value of $\Psi(x, t)$
  - ◇ Keep as much of the spectrum near k_0 (where $A(k)$ peaks)
  - ◇ Solution: Keep the phase $(kx - \omega(k)t)$ stationary

$$\frac{d}{dk}(kx - \omega(k)t)\Big|_{k=k_0} = 0$$

$$\Rightarrow \quad x - \frac{d\omega}{dk}\Big|_{k=k_0} t = 0$$

- Therefore, at $t \neq 0$, the wave packet is at

$$x = \frac{d\omega}{dk}\Big|_{k_0} t$$

  - ◇ Group velocity:

$$v_g \equiv \frac{d\omega}{dk}\Big|_{k_0} = \frac{x}{t} \neq v_p \quad \text{unless } \omega(k) \propto k \tag{7}$$

  - ◇ Particle: $v_g = p/m = \hbar k/m = d\omega/dk$
    - ▲ Integrating

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} + \text{const}$$
$$\hbar\omega = \frac{p^2}{2m} + \text{const} = E$$

▲ Note: $v_p \neq v_g$ (Warning!)

- Is this a consistent picture of a particle?

D. Example: Gaussian Wave packet

- Initially $(t = 0)$

$$\Psi(x, t = 0) = \frac{1}{(2\pi\sigma^2)^{1/4}} \mathrm{e}^{-x^2/4\sigma^2}$$

$$A(k) = \left(\frac{2\sigma^2}{\pi}\right)^{1/4} \mathrm{e}^{-(k-k_0)^2\sigma^2}$$

◇ Localized at $x = 0$ at $t = 0$

◇ Has momentum $p = \hbar k_0$

◇ Attribute the size of the particle to σ

- $t > 0$

$$\Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) \mathrm{e}^{i(kx-\omega_0 t)} dk$$

◇ Expand:

$$\begin{aligned} \omega(k) &= \omega(k_0) + \left.\frac{d\omega}{dk}\right|_{k_0} (k - k_0) + \frac{1}{2}\frac{d^2\omega}{dk^2}(k - k_0)^2 \\ &\equiv \omega_0 + v_g(k - k_0) + \beta(k - k_0)^2 \end{aligned}$$

◇ Let $k' \equiv k - k_0$

$$\begin{aligned} \Psi(x, t) &= \frac{1}{\sqrt{2\pi}} \left(\frac{2\sigma^2}{\pi}\right)^{1/4} \int_{-\infty}^{\infty} \mathrm{e}^{-k'^2\sigma^2} \mathrm{e}^{i[(k_0+k')x-\omega_0 t-v_g k' t-\beta k'^2 t]} dk' \\ &= \frac{1}{\sqrt{2\pi}} \left(\frac{2\sigma^2}{\pi}\right)^{1/4} \mathrm{e}^{i(k_0 x-\omega_0 t)} \int_{-\infty}^{\infty} \mathrm{e}^{-k'^2(\sigma^2+i\beta t)} \mathrm{e}^{ik'(x-v_g t)} dk' \\ &= \frac{1}{\sqrt{2\pi}} \left(\frac{2\sigma^2}{\pi}\right)^{1/4} \mathrm{e}^{i(k_0 x-\omega_0 t)} \sqrt{\frac{\pi}{\sigma'^2}} \mathrm{e}^{-(x-v_g t)^2/4\sigma'^2} \end{aligned}$$

▲ $k_0 x - \omega t =$ overall phase

▲ Wave is traveling at speed $x/t = v_g$

- Is our wave function a 'real' particle?

◇ Identify $|\sigma'|$ with the size of the particle

- ◇ e.g., Let $\sigma = 1$ fm for a proton (at $t = 0$)
- ◇ Examine $|\Psi(x,t)|^2$

$$|\Psi(x,t)|^2 = \frac{1}{2\pi}\sqrt{\frac{2\sigma^2}{\pi}}\frac{\pi}{\sqrt{\sigma^4+\beta^2t^2}}\exp\left[-(x-v_gt)^2/2(\sigma^2+\beta^2t^2/\sigma^2)\right]$$

- The Gaussian is spreading!!

$$\sigma_x \equiv \sqrt{\sigma^2+\beta^2t^2/\sigma^2}$$

- ◇ Smaller it starts $\Rightarrow$ Faster it spreads!
- ◇ Proton: $mc^2 = 938$ MeV
- ◇ $c\hbar = 200$ MeV·fm, $c = 3\times10^{14}$ fm/ns

$$\begin{aligned}\sigma(t) &= \sigma_0\left[1+\left(\frac{\hbar}{2m}\right)^2\frac{t^2}{\sigma_0^4}\right]^{\frac{1}{2}}\\ &= 3\times10^{13}\ t \text{ fm/ns}\\ &= 3t \text{ cm/ns}\end{aligned}$$

- ◇ After 1ns, the particle is $>$ 1cm !!
- ◇ All because the wave packets have different momentum ($v_p \neq v_g$)

E. Interpreting the Wave Function

- Max Born
  - ◇ $|\Psi(x,t)|^2dx$ = The *probability* of finding the particle in the interval $x + dx$ at time t
  - ◇ Probabilistic description of physics!
- Advantages
  - ◇ Agrees with fact (matches experiment)
  - ◇ Evolution of $\Psi(x)$ is well defined
  - ◇ Ψ contains all possible information about the particle
- Consequences
  - ◇ $\int_{-\infty}^{\infty}|\Psi(x,t)|^2dx = 1$
  - ◇ Must deal with probabilities and averages

F. Schrodinger Equation

- Start with plane waves (free particles)

$$\Psi(x,t) \sim \mathrm{e}^{i(kx-\omega t)} = \exp\left[\frac{i}{\hbar}(px - Et)\right]$$

$$E = p^2/2m \Rightarrow \hbar\omega = \frac{\hbar^2 k^2}{2m}$$

- Postulate

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}$$

- Forces?
  - ◇ Consider conservative forces (time independent)

$$F = -\nabla V(\mathbf{r})$$

  - ◇ $\Rightarrow$ $E = p^2/2m + V(r)$ or $\hbar\omega = \hbar^2 k^2/2m + V(r)$

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V(r)\Psi \tag{8}$$

G. Fundamentals of Wave Mechanics (Postulates)

(a) Any physically-realizable state of a particle has associated with it a state function $\Psi(\mathbf{r},t)$ that contains all observable information

(b) $|\Psi(\mathbf{r},t)|^2 d^3\mathbf{r}$ is the probability of finding the particle in a volume $d^3\mathbf{r}$ around position $\mathbf{r}$ at time t

(c) The time dependence of $\Psi(\mathbf{r},t)$ is given by the Schrodinger Equation

III. Dirac QM (Bra-Ket Formalism)

A. Stern-Gerlach experiment (1921)

- Silver atoms: Z=47
  - ◇ Simplify the atomic structure
    - ▲ Z=46 $\sim$ closed shell
    - ▲ $\Rightarrow$ 1 free electron (5s)
- Magnetic moment: $\mu_{Ag} \propto$ Spin of 1 electron

$$F_z = \frac{\partial}{\partial z}(\vec{\mu} \cdot \vec{B}) = \mu_z \cdot \frac{\partial B}{\partial z}$$

- Predict trajectory
  - ◇ Atoms with $\vec{\mu}$ pointing up ($S_z < 0$) go down
  - ◇ Atoms with $\vec{\mu}$ pointing down ($S_z > 0$) go up
- Predict pattern at detector

- Quantum Mechanics
  - ◇ Quantization of electron spin

$$S_z = \pm\hbar/2$$

  - ◇ Keep in mind:
    - ▲ Nothing special about the $\hat{z}$-axis
    - ▲ Could quantize x or y components too
- Sequential Stern-Gerlach experiments
  - ◇ Key: Cannot simultaneously measure S_x, S_z
  - ◇ Anti-commutative nature of QM

B. Bra-Ket Notation

- $|\alpha\!>, |\beta\!>, ...$
- Mathematics: Complex vector space whose dimensionality is determined by the physical nature of the system
  - ◇ Spin: Finite dimensions
  - ◇ Position: Infinite dimensions (Hilbert space)
- Basic rules

$$c|\alpha\!> = |\alpha\!>c$$

  - ◇ c: complex number
  - ◇ $|\alpha\!>$ is a physical state which has remained unchanged

$$|\alpha> + |\beta> = |\gamma>$$

C. Eigenkets:

- Consider an observable A
- In general,

$$A|\alpha> \neq c|\alpha>$$

- *But* $\exists$ a space of eigenkets

$$|a> = \{|a'>, |a''>, |a'''>, ...\}$$

  ◇ such that

$$A|a'> = a'|a'>, \quad (9)$$
$$A|a''> = a''|a''>, \quad (10)$$
$$A|a'''> = a'''|a'''> \quad (11)$$

  ◇ with $a', a'', \ldots$ eigenvalues

- Example: Spin 1/2 system

$$S_z|S_z;+> = \frac{\hbar}{2}|S_z;+>$$
$$S_z|S_z;-> = -\frac{\hbar}{2}|S_z;->$$

  ◇ Matrix form

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

  ◇ Similarly, $S_x|S_x;\pm> = \pm\frac{\hbar}{2}|S_x;\pm>$

- KEY: Any ket $|\alpha>$ can be described as a sum of eigenkets

$$|\alpha> = \sum_{a'}^{N} g_{a'}|a'> \quad (12)$$

  ◇ Infinite sum (integral) for continuous observables

- $\diamond$ $N = 2$ for a spin 1/2 system

- Completeness Relation

$$\sum_{a'} |a'\rangle\langle a'| = 1 \tag{13}$$

D. Bra space

$$\langle\alpha|, \langle\beta|, ...$$

- Mirror image of ket space $\Rightarrow$ one-to-one correspondence

$$|\alpha\rangle \Leftrightarrow \langle\alpha|$$

$$|a'\rangle, |a''\rangle \Leftrightarrow \langle a'|, \langle a''|$$

- Mirror

$$c|\alpha\rangle \Leftrightarrow c^*\langle\alpha|$$

E. Inner product

$$\langle\beta|\alpha\rangle = \text{complex number}$$

$$\therefore \langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*$$

- Implications for $\langle\alpha|\alpha\rangle$?

$$\langle\alpha|\alpha\rangle = \langle\alpha|\alpha\rangle^*$$

$$\Rightarrow \langle\alpha|\alpha\rangle \quad \text{is a real number}$$

- *Postulate*

$$\langle\alpha|\alpha\rangle \geq 0$$

- $\diamond$ Recall the probabilistic interpretation of $|\Psi|^2 d^3r$

F. Wave/Bra-Ket Correspondence

Wave	Bra-ket
Ψ	$\|\alpha>$
Ψ^*	$<\alpha\|$
$\int \Psi^*\Psi$	$<\alpha\|\alpha>$
$\int \Psi^* A\Psi$	$<\alpha\|A\|\alpha>$

- $\Psi = <x|\alpha>$

G. Operator: $X|\alpha>$

- Operators are additive

$$X + Y = Y + X$$

- but non-commutative

$$XY \neq YX$$

$$[X, Y] \neq 0$$

- Observable: Desire the eigenvalues of X are real (Hermetian)

$$\Rightarrow \; X = X^\dagger$$

- Theorem: The eigenvalues of a Hermetian operator A are real; the eigenkets of A correspond to different eigenvalues are orthogonal.
  - ◇ Proof:
    - ▲ First

$$A|a'> = a'|a'>$$

$$\begin{aligned} <a''|A &= (A^\dagger|a''>)^\dagger \\ &= (a''|a''>)^\dagger \\ &= <a''|a''^* \end{aligned}$$

    - ▲ Consider

$$\begin{aligned} <a''|A|a'> - <a''|A|a'> = 0 \\ <a''|a'>a' - a''^*<a''|a'> = 0 \end{aligned}$$

$$(a' - a''^*)<a''|a'> = 0 \tag{14}$$

▲ Option (i) $a'' = a'$

$$\Rightarrow\ a' - a''^* = 0$$
$$\Rightarrow\ a' = a'^* \quad \text{(Real eigenvalue)}$$

▲ Option (ii) $a' \neq a''$

$$\Rightarrow\ <a''|a'> = 0 \quad \text{(Orthogonal eigenstates)}$$

- Operator

$$A = \sum_{a'} a'\ |a'><a'|$$

H. Measurements

- Dirac: "A measurement always causes the system to jump into an eigenstate of the dynamical variable that is being measured [and one records the eigenvalue]."

$$|\alpha> \rightarrow |a'>, |a''>, |a'''>$$

  - ◇ Probability of measuring a'

$$c_{a'} = |<a'|\alpha>|^2 \tag{15}$$

  - ◇ In general, the process of making a measurement changes the state
  - ◇ Fundamental Postulate! (no proof)

- Expectation values

$$< A > \equiv\ <\alpha|A|\alpha> \tag{16}$$

  - ◇ Not a single measurement but the 'average' of an ensemble

- Example: Spin 1/2 system
  - ◇ Recall

  - ◇ Normalization ($\sum |\text{states}|^2 = 1$) requires:

$$|{<}S_z;+|S_x;+{>}| = |{<}S_z;-|S_x;+{>}| = \frac{1}{\sqrt{2}}$$

$$\Rightarrow\ |S_x;+{>} = \frac{1}{\sqrt{2}}|+{>} + \frac{1}{\sqrt{2}}\mathrm{e}^{i\delta_1}|-{>}$$

- ▲ δ_1 is real and provides an arbitrary phase

◇ How about $|S_x;-{>}$?

- ▲ Must be orthogonal to $|S_x;+{>}$

$$\Rightarrow\ |S_x;-{>} = \frac{1}{\sqrt{2}}|+{>} - \frac{1}{\sqrt{2}}\mathrm{e}^{-i\delta_1}|-{>}$$

◇ Construct the S_x operator

$$\begin{aligned} S_x &= \sum_{a'} a'|a'{>}{<}a'| \\ &= \frac{\hbar}{2}\left(\,|S_x;+{>}{<}S_x;+| \ - \ |S_x;-{>}{<}S_x;-|\,\right) \\ &= \frac{\hbar}{2}\left[\,\left(\mathrm{e}^{-i\delta_1}|+{>}{<}-|\right) \ + \ \left(\mathrm{e}^{i\delta_1}|-{>}{<}+|\right)\right] \end{aligned}$$

◇ Is S_x Hermetian? Yup.., $S_x = S_x^\dagger$

◇ S_y is constructed in similar fashion

$$S_y = \frac{\hbar}{2}\left[\,\left(\mathrm{e}^{-i\delta_2}|+{>}{<}-|\right) \ + \ \left(\mathrm{e}^{i\delta_2}|-{>}{<}+|\right)\right]$$

◇ Can we determine δ_1, δ_2?

- ▲ There is nothing special about $\hat{z}$
- ▲ Could replace $z \to y$

$$|{<}S_y;\pm|S_x;+{>}| = |{<}S_y;\pm|S_x;+{>}| = \frac{1}{\sqrt{2}}$$

$$\Rightarrow\ \frac{1}{2}|1 \pm \mathrm{e}^{i(\delta_1-\delta_2)}| = \frac{1}{\sqrt{2}}$$

- ▲ Therefore: $\quad \delta_1 - \delta_2 = \pi/2$
- ▲ Choose: $\quad \delta_1 = 0, \delta_2 = \pi/2$

◇ Summarizing:

$$
\begin{aligned}
&|S_z;\pm\rangle = |\pm\rangle \\
&|S_x;\pm\rangle = \frac{1}{\sqrt{2}}|+\rangle \pm \frac{1}{\sqrt{2}}|-\rangle \\
&|S_y;\pm\rangle = \frac{1}{\sqrt{2}}|+\rangle \pm \frac{i}{\sqrt{2}}|-\rangle \\
&S_x = \frac{\hbar}{2}\left[\,(|+\rangle\langle -|) + (|-\rangle\langle +|)\,\right] = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\
&S_y = \frac{\hbar}{2}\left[\,-i(|+\rangle\langle -|) + i(|-\rangle\langle +|)\,\right] = \frac{i\hbar}{2}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \\
&S_z = \frac{\hbar}{2}\left[\,(|+\rangle\langle +|) - (|-\rangle\langle -|)\,\right] = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\end{aligned}
$$

- Aside on angular momentum
  - ◇ Commutating

$$[S_i, S_j] = i\varepsilon_{ijk}\hbar S_k$$

  - ◇ Total angular momentum

$$S^2 \equiv S_x^2 + S_y^2 + S_z^2 = \frac{3}{4}\hbar^2$$

  - ◇ Another commutation relation

$$[S^2, S_i] = 0$$

I. (In)Compatible Observables

- Compatible: $[A, B] = 0$
- Theorem: If A, B are compatible, the matrix elements $\langle a''|B|a'\rangle$ are all diagonal.
  - ◇ $|a'\rangle$ are simultaneous eigenkets of A and B

$$\langle a'|B|a'\rangle = b$$

  - ◇ Tend to denote the eigenket as $|a', b'\rangle$
  - ◇ Important theorem for perturbation theory (especially degenerate)
- Example: Angular momentum
  - ◇ L^2, L_z are compatible

$$L^2|\ell, m\rangle = \ell(\ell+1)\hbar^2|\ell, m\rangle \tag{17}$$

$$L_z|\ell, m\rangle = m\hbar|\ell, m\rangle \tag{18}$$

- Incompatible: $[A, B] \neq 0$
  - ◇ Incompatible observables do not have a complete set of simultaneous observables
  - ◇ Sequential selective measurements

  (Fig 1.7; Sakurai)

J. Uncertainty Relation

- Define an operator

$$\Delta A \equiv A - < A >$$

- Dispersion: The expectation of $(\Delta A)^2$

$$< (\Delta A)^2 > = < A^2 > - < A >^2$$

  - ◇ Characterizes the 'fuzziness' of an observable
  - ◇ e.g., $< (\Delta S_x)^2 >$ for a $|+>$ state is $\hbar^2/4$

- Theorem:

$$< (\Delta A)^2 >< (\Delta B)^2 > \geq \frac{1}{4} | < [A, B] > |^2$$

  - ◇ *Lemma 1:* Schwarz inequality

$$<\alpha|\alpha><\beta|\beta> \geq |<\alpha|\beta>|^2$$

$$|a|^2 |b|^2 \geq |a \cdot b|^2$$

  - ◇ *Lemma 2:* The expectation value of a Hermitian operator is purely real
  - ◇ *Lemma 3:* The expectation value of an anti-Hermetian operator, defined by $C = -C^\dagger$ is purely imaginary

- Proof
  - ◇ Schwarz inequality

$$< (\Delta A)^2 >< (\Delta B)^2 > \geq | < \Delta A \Delta B > |^2$$

◇ Consider

$$\Delta A \Delta B = \frac{1}{2}[\Delta A, \Delta B] + \frac{1}{2}\{\Delta A, \Delta B\}$$
$$[\Delta A, \Delta B] = [A, B]$$

◇ Therefore

$$< \Delta A \Delta B > = \frac{1}{2} < [A, B] > + \frac{1}{2} < \{A, B\} >$$

▲ $< [A, B] >$ is purely imaginary

▲ $< \{A, B\} >$ is purely real

◇ Therefore

$$| < \Delta A \Delta B > |^2 = \frac{1}{4}| < [A, B] > |^2 + \frac{1}{4}| < \{\Delta A, \Delta B\} > |^2$$

K. Position, Momentum, and Translation

- Continuous spectra
  - ◇ Infinite range of eigenvalues
  - ◇ Replace sums by integrals

$$\sum_{a'} |a'><a'| = 1 \ \rightarrow \ \int d\xi' |\xi'><\xi'| = 1$$

$$<a''|A|a'> = a'\delta_{a',a''} \rightarrow <\xi''|\xi|\xi'> = \xi'\delta(\xi'' - \xi')$$

- Position operator with usual eigenvalue and eigenkets

$$x|x'> = x'|x'>$$

- Can express any state as

$$|\alpha> = \int_{-\infty}^{\infty} dx' |x'><x'|\alpha>$$

  - ◇ Interpretation: Probability of being within $x' \pm dx'$
    - ▲ $|<x'|\alpha>|^2 dx'$
    - ▲ Analogous to our discrete eigenkets
  - ◇ Extending to 3D

$$|\alpha> = \int d^3x' |\mathbf{x}'><\mathbf{x}'|\alpha>$$

- ▲ $|\mathbf{x}'\rangle$ is a simultaneous eigenket of observables x, y, z

$$|\mathbf{x}'\rangle = |x', y', z'\rangle$$

- ▲ Implicit: $[x_i, x_j] = 0$

• Translation: $\mathcal{T}(x)$ (Motivating momentum)

◇ Start with a state localized at x'

◇ Introduce an operator which changes the state to one localized at $x' + dx'$

$$\mathcal{T}(dx')|x'\rangle = |x' + dx'\rangle$$

- ▲ $|x'\rangle$ is not an eigenket of $\mathcal{T}$

◇ Properties of $\mathcal{T}$

(a) Unitarity $\mathcal{T}^\dagger(dx)\mathcal{T}(dx) = 1$

- ▲ Conservation of probability
- ▲ If $|\alpha\rangle$ is normalized to unity, desire $\mathcal{T}|\alpha\rangle$ is too.

(b) Consider successive translations dx', dx''

$$\mathcal{T}(dx'')\mathcal{T}(dx') = \mathcal{T}(dx' + dx'')$$

(c) Translation in the opposite direction should be the inverse of the original

$$\mathcal{T}(-dx') = \mathcal{T}^{-1}(dx')$$

(d) As $dx' \to 0, \mathcal{T} \to 1$

$$\lim_{dx' \to 0} \mathcal{T}(dx') = 1$$

◇ Solution: (Ansatz)

$$\mathcal{T}(d\mathbf{x}') = 1 - i\mathbf{K} \cdot d\mathbf{x}'$$

- ▲ Components of $\mathbf{K}$ (i.e. K_x, K_y, K_z) are Hermitian operators
- ▲ Properties (a)-(d) are satisfied to 1st order in dx'

◇ $\mathbf{K}, \mathbf{x}$ commutation

- ▲ Consider

$$x\mathcal{T}(dx')|x'\rangle = x|x' + dx'\rangle = (x' + dx')|x' + dx'\rangle$$

- ▲ Also

$$\mathcal{T}(dx')x|x'\rangle = x'|x' + dx'\rangle$$

$$\Rightarrow\ [x, \mathcal{T}(x')]|x'\rangle = dx'|x' + dx'\rangle \approx dx'|x'\rangle$$

▲ Continuing..

$$[x, \mathcal{T}(x')] = dx' \tag{19}$$
$$-i\mathbf{x}\,\mathbf{K}\cdot d\mathbf{x}' + i\mathbf{K}\cdot d\mathbf{x}'\,\mathbf{x} = d\mathbf{x}' \tag{20}$$

▲ Choose $d\mathbf{x}'$ in the direction $\hat{x}_j$

$$[x_i, K_j] = i\delta_{ij}$$

- Momentum (Identifying $\mathbf{K}$)
  - ◇ In classical mechanics, momentum generates translation
  - ◇ 'Generating Function': $F(x,p) = \mathbf{x}\cdot\mathbf{p} + \mathbf{p}\cdot d\mathbf{x}$
  - ◇ Set

$$\mathbf{K} = \frac{\mathbf{p}}{\text{constant of dimension of action}}$$

▲ de Broglie

▲ Constant is $\hbar$

  - ◇ Therefore

$$\mathcal{T}(dx') = 1 - i\mathbf{p}\cdot d\mathbf{x}'/\hbar$$

$$[x_i, p_j] = i\hbar\delta_{ij}$$

  - ◇ x, p are incompatible observables

$$<(\Delta x)^2><(\Delta p)^2> \geq \hbar^2/4$$

- Finite translation Δx

$$\mathcal{T}(\Delta x\hat{x})|\mathbf{x}'> = |\mathbf{x}' + \Delta x'\hat{x}>$$

  - ◇ Successive (N) infinitesimal translations with $dx' = \Delta x/N$

$$\mathcal{T}(\Delta x'\hat{x}) = \lim_{N\to\infty}\left(1 - \frac{ip_x\Delta x'}{N\hbar}\right)^N \tag{21}$$
$$= \exp\left(-\frac{ip_x\Delta x'}{\hbar}\right) \tag{22}$$

▲ Note: p_x is an operator

L. Wave Functions (Return at last)

- Position-space wave function

- ◇ Recall

$$|\alpha\rangle = \int dx' |x'\rangle\langle x'|\alpha\rangle$$

- ◇ Identify

$$\Psi_\alpha(x') = \langle x'|\alpha\rangle$$

  - ▲ $\Psi_\alpha(x')$ is an expansion coefficient just like $\langle a'|\alpha\rangle$
  - ▲ Probabilistic interpretation of $\Psi(x')$ is built in (not postulated!)

- ◇ Inner product

$$\begin{aligned}\langle\beta|\alpha\rangle &= \int dx' \langle\beta|x'\rangle\langle x'|\alpha\rangle \\ &= \int dx' \Psi^*_\beta(x')\Psi_\alpha(x')\end{aligned}$$

  - ▲ $\langle\beta|\alpha\rangle$ characterizes the overlap between two wave functions
  - ▲ Probability amplitude for state $|\alpha\rangle$ to be found in state $|\beta\rangle$

- ◇ Position operator $f(x)$

$$\langle\beta|f(x)|\alpha\rangle = \int dx' \Psi^*_\beta(x') f(x') \Psi_\alpha(x')$$

• Momentum operator in position basis

- ◇ Consider an infinitesimal translation $\delta x'$

$$\begin{aligned}(1 - \frac{ip\delta x'}{\hbar})|\alpha\rangle &= \int dx' \mathcal{T}(\delta x')|x'\rangle\langle x'|\alpha\rangle && (23)\\ &= \int dx' |x' + \delta x'\rangle\langle x'|\alpha\rangle && (24)\\ &= \int dx' |x'\rangle\langle x' - \delta x'|\alpha\rangle && (25)\\ &= \int dx' |x'\rangle \left(\langle x'|\alpha\rangle - \delta x' \frac{\partial}{\partial x'}\langle x'|\alpha\rangle \right) && (26)\end{aligned}$$

- ◇ Altogether

$$p|\alpha\rangle = \int dx' |dx'\rangle \left(-i\hbar \frac{\partial}{\partial x}\langle x'|\alpha\rangle \right)$$

$$\langle x'|p|\alpha\rangle = -i\hbar \frac{\partial}{\partial x}\langle x'|\alpha\rangle$$

- ◇ Similarly

$$\langle\beta|p|\alpha\rangle = \int dx' \Psi^*_\beta(x') \left(-i\hbar \frac{\partial}{\partial x'} \right) \Psi_\alpha(x')$$

- ▲ Note: we have derived (not postulated) this relation from the concept of momentum

- Momentum-space wave function
  - ◇ Standard eigenkets and eigenvalues

$$p|p'\rangle = p'|p'\rangle$$

    - ▲ Complete set of eigenkets

$$|\alpha\rangle = \int dp'|p'\rangle\langle p'|\alpha\rangle$$

    - ▲ Identify $\phi_\alpha(p') = \langle p'|\alpha\rangle$
  - ◇ How do the x and p representations correspond?
    - ▲ Recall: A unitary operator U exists which transforms between the two spaces

$$\langle a^k|U|a^l\rangle = \langle a^k|b^l\rangle$$

    - ▲ Examine $\langle x'|p'\rangle$
    - ▲ Consider $\langle x'|p|p'\rangle$
      - ○ Apply p to x'

$$\langle x'|p|p'\rangle = -i\hbar\frac{\partial}{\partial x}\langle x'|p'\rangle$$

      - ○ Apply p to p'

$$\langle x'|p|p'\rangle = p'\langle x'|p'\rangle$$

      - ○ Solving the differential equation

$$\langle x'|p'\rangle = N\exp\left(\frac{ip'x'}{\hbar}\right)$$

      - ○ The plane wave returns!!
      - ○ Solve for N by demanding $\langle x'|x''\rangle = \delta(x''-x')$

$$\langle x'|p'\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp\left(\frac{ip'x'}{\hbar}\right)$$

  - ◇ Our transformation equations:

$$\Psi_\alpha(x') = \frac{1}{\sqrt{2\pi\hbar}}\int dp'\exp\left(\frac{ip'x'}{\hbar}\right)\phi_\alpha(p') \qquad (27)$$

$$\phi_\alpha(p') = \frac{1}{\sqrt{2\pi\hbar}}\int dx'\exp\left(\frac{-ip'x'}{\hbar}\right)\Psi_\alpha(x') \qquad (28)$$

III. Quantum Dynamics

A. Time Evolution

- In non-relativistic QM, time is a parameter
  - ◇ x, p are operators
  - ◇ Even in relativistic QM, time is a parameter (so is position!)
- Time Evolution operator
  - ◇ Let $|\alpha, t_0; t\rangle$ be our state ket $|\alpha\rangle$ at t_0 which has evolved to a later time t
  - ◇ Require: $|\alpha, t_0; t_0\rangle = |\alpha\rangle$
  - ◇ Introduce an operator $\mathcal{U}$

$$|\alpha, t_0; t\rangle = \mathcal{U}(t, t_0)|\alpha\rangle$$

  - ▲ Unitary: $\mathcal{U}\mathcal{U}^\dagger = 1$
    - ∘ Probability conservation
    - ∘ $\sum_{a'} |c_{a'}(t)|^2 = \sum_{a'} |c_{a'}(t_0)|^2$
    - ∘ But expect $|c_{a'}(t)| \neq |c_{a'}(t_0)|$
  - ▲ Composite: $\mathcal{U}(t_2, t_0) = \mathcal{U}(t_2, t_1)\mathcal{U}(t_1, t_0)$
  - ▲ Infinitesimal evolution:

$$\lim_{dt \to 0} \mathcal{U}(t_0 + dt, t_0) = 1$$

- Assert

$$\mathcal{U}(t_0 + dt, t_0) = 1 - i\Omega dt$$

  - ◇ What is Ω?
    - ▲ Ω is Hermetian (to satisfy unitarity of $\mathcal{U}$)
    - ▲ Ω has dimension of frequency
    - ▲ Borrow from classical mechanics that the Hamiltonian generates time evolution (e.g. Goldstein)

$$\Omega = H/\hbar$$

      - ∘ Is this the same as the $\hbar$ in our momentum definition?
      - ∘ It must be if we wish QM to give sensible relations in the classical limit!
  - ◇ Altogether:

$$\mathcal{U}(t_0 + dt, t_0) = 1 - \frac{iHdt}{\hbar} \tag{29}$$

B. Schrodinger Equation

- The composite property of $\mathcal{U}$ implies:

$$\mathcal{U}(t+dt,t_0) = \mathcal{U}(t+dt,t)\mathcal{U}(t,t_0) = \left(1 - \frac{iHdt}{\hbar}\right)\mathcal{U}(t,t_0)$$

$$\mathcal{U}(t+dt,t_0) - \mathcal{U}(t,t_0) = -\frac{iH}{\hbar}\mathcal{U}(t,t_0)\ dt$$

- Schrodinger equation for $\mathcal{U}$:

$$i\hbar\frac{\partial}{\partial t}\mathcal{U}(t,t_0) = H\mathcal{U}(t,t_0) \tag{30}$$

- Schrodinger equation for a state ket

$$i\hbar\frac{\partial}{\partial t}\mathcal{U}(t,t_0)|\alpha> = H\mathcal{U}(t,t_0)|\alpha>$$

  ◇ $|\alpha>$ has no time dependence

$$i\hbar\frac{\partial}{\partial t}|\alpha,t_0;t> = H|\alpha,t_0;t> \tag{31}$$

- To determine all time evolution, it is sufficient to derive $\mathcal{U}$ and apply it to $|\alpha>$

  (a) *Case 1:* H is independent of t

$$\mathcal{U}(t,t_0) = \exp\left[\frac{-iH(t-t_0)}{\hbar}\right] \tag{32}$$

  (b) *Case 2:* H is time dependent but $[H(t),H(t_0)] = 0$

$$\mathcal{U}(t,t_0) = \exp\left[-\left(\frac{i}{\hbar}\right)\int_{t_0}^{t} dt' H(t')\right] \tag{33}$$

  (c) *Case 3:* $[H(t),H(t_0)] \neq 0$

$$\mathcal{U}(t,t_0) = 1 + \sum_{n=1}^{\infty}\left(\frac{-i}{\hbar}\right)^n \int_{t_1}^{t_2} dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_{n-1}} dt_n H(t_1)H(t_2)\ldots H(t_n) \tag{34}$$

C. Energy Eigenkets

- Consider our $\{|a'>\}$ basis
- If $[A,H] = 0$, then $|a'>$ are a set of energy eigenkets

$$H|a'> = E_{a'}|a'>$$

◇ Applying the time-evolution operator in the a' basis

$$\mathcal{U} = \exp\left[\frac{-iHt}{\hbar}\right] = \sum_{a'}\sum_{a''} |a''\rangle\langle a''| \exp(\frac{-iHt}{\hbar})|a'\rangle\langle a'| \tag{35}$$

$$= \sum_{a'} |a'\rangle \exp(\frac{iE_{a'}t}{\hbar})\langle a'| \tag{36}$$

◇ Only need to know our initial state $|\alpha\rangle$ in terms of the a' basis

$$|\alpha\rangle = \sum_{a'} c_{a'}|a'\rangle$$

▲ Time evolve

$$|\alpha, t_0; t\rangle = \mathcal{U}(t, t_0)|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \exp\left(\frac{-iE_{a'}t}{\hbar}\right) \tag{37}$$

- Stationary state
  - ◇ What if $|\alpha\rangle = |a'\rangle$?

$$|\alpha, t_0; t\rangle = |a'\rangle \exp\left(\frac{-iE_{a'}t}{\hbar}\right)$$

  - ◇ $|a'\rangle$ is a constant of the motion
- In general, multiple observables may commute with H and A

$$[A, B] = [B, C] = \ldots 0$$

$$[A, H] = [B, H] = \ldots 0$$

  - ◇ Express our initial state in terms of eigenstates of $A, B, C, \ldots$
  - ◇ Time-evolution is explicit
- Time dependence of expectation values
  - ◇ Eigenstate of A: $|a'\rangle$

$$|a', t_0; t\rangle = \mathcal{U}(t, t_0)|a'\rangle$$

▲ At time t, operator B has expectation value

$$< B > = \left(\langle a'|\mathcal{U}^\dagger\right) B \left(\mathcal{U}|a'\rangle\right) \tag{38}$$

$$= \left[\langle a'| \exp\left(\frac{iE_{a'}t}{\hbar}\right)\right] B \left[\exp\left(\frac{-iE_{a'}t}{\hbar}\right)|a'\rangle\right] \tag{39}$$

$$= \langle a'|B|a'\rangle \tag{40}$$

▲ Independent of t

▲ Stationary state

◇ Consider $|\alpha\!> = \sum_{a'} c_{a'} |a'\!>$

$$< B > = \left[\sum_{a'} c^*_{a'} \!<\! a'| \exp\left(\frac{iE_{a'}t}{\hbar}\right) \right] B \left[\sum_{a''} c_{a''} \exp\left(\frac{-iE_{a''}t}{\hbar}\right) |a''\!> \right] \quad (41)$$

$$= \sum_{a'} \sum_{a''} c^*_{a'} c_{a''} \!<\! a'|B|a'\!> \exp\left[\frac{-i(E_{a''} - E_{a'})t}{\hbar}\right] \quad (42)$$

▲ Oscillating terms

▲ Angular frequency

$$\omega_{a''a'} \equiv \frac{(E_{a''} - E_{a'})}{\hbar} \quad (43)$$

D. An Example (At last!)

- Spin procession of a spin 1/2 system
- Magnetic moment: $\mu = e\hbar/2m_e c$ in external B field

$$H = -\vec{\mu} \cdot \vec{B} = -\left(\frac{e}{m_e c}\right) \vec{S} \cdot \vec{B}$$

◇ Take $\vec{B} = B\hat{z}$

◇ $H = -\left(\frac{eB}{m_e c}\right) S_z$

- Obviously, $[H, S_z] = 0$

◇ S_z eigenstates are energy eigenstates ($|+\!>, |-\!>$)

◇ Energy eigenvalues

$$E_{\pm} = \mp \frac{e\hbar B}{2m_e c} \quad \text{for } S_z \pm$$

◇ Define $\omega \equiv \frac{|e|B}{m_e c} = \Delta E/\hbar$

$$H = \omega S_z$$

- Time operator

$$\begin{aligned} \mathcal{U}(t,0) &= \exp\left(\frac{-iHt}{\hbar}\right) \\ &= \exp\left(\frac{-i\omega S_z t}{\hbar}\right) \end{aligned}$$

- Consider an arbitrary initial state

$$|\alpha\rangle = c_+|+\rangle + c_-|-\rangle$$

  - ◇ At time t

$$\begin{aligned}|\alpha, t_0 = 0; t\rangle &= \mathcal{U}|\alpha\rangle \\ &= c_+ \exp(-i\omega t/2)|+\rangle \;+\; c_- \exp(i\omega t/2)|-\rangle\end{aligned}$$

  - ◇ Consider, $c_+ = 1, c_- = 0$

$$|\alpha, t_0 = 0; t\rangle = \exp(-i\omega t/2)|+\rangle$$

    - ▲ Stationary state
    - ▲ Remains in $|+\rangle$ always

- Let the initial state be $|S_x; +\rangle$
  - ◇ Recall

$$|\alpha\rangle = |S_x; +\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|-\rangle$$

  - ◇ At $t = 0$,

$$|\langle S_x; +|\alpha\rangle|^2 = |\langle S_x; +|S_x; +\rangle|^2 = 1$$

  - ◇ How about at time t?

$$|\alpha, t_0 = 0; t\rangle = \mathcal{U}(t, 0)|\alpha\rangle$$

$$\begin{aligned}\left|\langle S_x; +|\alpha, t_0 = 0; t\rangle\right|^2 &= \left|\left[\frac{1}{\sqrt{2}}\langle +| + \frac{1}{\sqrt{2}}\langle -|\right]\left[\frac{1}{\sqrt{2}}\exp\frac{-i\omega t}{2}|+\rangle + \frac{1}{\sqrt{2}}\exp\frac{i\omega t}{2}|-\rangle\right]\right|^2 \\ &= \left|\frac{1}{2}\exp\frac{-i\omega t}{2} + \frac{1}{2}\exp\frac{i\omega t}{2}\right|^2 \\ &= \cos^2\frac{\omega t}{2}\end{aligned}$$

    - ▲ Similarly,

$$|\langle S_x; -|\alpha, t_0 = 0; t\rangle|^2 = \sin^2\frac{\omega t}{2}$$

    - ▲ Finite probability for S_x- !!
    - ▲ S_x is precessing in time in $x - y$ plane

- Expectation value

$$\begin{aligned}
< S_x > &= <\alpha, t_0 = 0; t|S_x|\alpha, t_0 = 0; t> \\
&= \sum\sum <\alpha, t_0 = 0; t|S_x; \pm><S_x; \pm|S_x|S_x; \pm><S_x; \pm|\alpha, t = 0; t> \\
&= \sum c_{S_x\pm}|<\alpha, t_0 = 0; t|S_x; \pm>|^2 \\
&= \frac{\hbar}{2}\cos^2\frac{\omega t}{2} - \frac{\hbar}{2}\sin^2\frac{\omega t}{2} \\
&= \frac{\hbar}{2}\cos\omega t
\end{aligned}$$

  ◇ Similarly

$$< S_y > = \frac{\hbar}{2}\sin\omega t \tag{44}$$

$$< S_z > = 0 \tag{45}$$

E. Time-Energy Uncertainty relation

- Correlation amplitude: Overlap between initial state $|\alpha>$ and its time evolved state $|\alpha, t_0 = 0; t>$

$$C(t) = <\alpha|\alpha, t_0 = 0; t> \tag{46}$$

$$= <\alpha|\mathcal{U}|\alpha> \tag{47}$$

  ◇ Modulus measures the resemblance of the two states

- Stationary state (eigenket)

$$C(t) = \exp\left(\frac{-iE_{a'}t}{\hbar}\right) \tag{48}$$

$$|C(t)| = 1 \tag{49}$$

- General situation

$$C(t) = \sum_{a'}|c_{a'}|^2\exp\frac{-iE_{a'}t}{\hbar}$$

  ◇ Sum of oscillating terms

  ◇ Expect $C(t)$ to decrease in time

- Continuous eigenenergies

$$C(t) = \int dE|A(E)|^2 g(E) \exp\left(\frac{-iEt}{\hbar}\right)$$

  - $A(E)$ = amplitude of state ($c_{a'}$)
  - $g(E)$ = density of eigenstates
  - Require $\int dE|A(E)|^2 g(E) = 1$

- Consider a system with $E = E_0 \pm \Delta E$

$$C(t) = \exp\left(\frac{-iE_0 t}{\hbar}\right) \int dE|A(E)|^2 g(E) \exp\left[\frac{-i(E-E_0)t}{\hbar}\right]$$

  - As t grows, the integral oscillates rapidly unless $|E - E_0| \ll \hbar/t$
  - If the interval where $|E - E_0| \approx \hbar/t$ is much narrower than ΔE, then $C(t) \to 0$ due to strong cancellations

- $C(t)$ departs from unity at time

$$t \approx \hbar/\Delta E$$

  - Regrouping

$$\Delta t \Delta E \approx \hbar$$

  - Spin 1/2
    - ▲ $<S_x;+|\alpha, t_0 = 0; t>$ becomes small when
    - ▲ $t \sim 1/\omega = \hbar/\Delta E$

- Energy-Time Uncertainty is fundamentally different from position momentum
  - This was obvious from the beginning? time, E are not operators
  - These concepts will return with stimulated emission

F. Schrodinger vs. Heisenberg

- Until now, we have adopted the Schrodinger picture
  - Time evolution operator acting on state kets
  - Observables (operators) are constant with time

- Heisenberg
  - State kets are constant
  - Observables evolve

- Consider evolution of an operator using a unitary transformation

$$<\beta|X|\alpha> \to \left(<\beta|U^\dagger\right) \cdot X \cdot \left(U|\alpha>\right) = <\beta|\left(U^\dagger X U\right)|\alpha>$$

- $\diamond$ Schrodinger: $|\alpha\rangle \to U|\alpha\rangle$
- $\diamond$ Heisenberg: $X \to U^\dagger X U$

- Key: Heisenberg conforms more closely with the techniques of classical physics
  - $\diamond$ Observables $\mathbf{x}, \mathbf{L}$ evolve in time
  - $\diamond$ Take $U \to \mathcal{U}$, the time-evolution operator
- Heisenberg equation of motion for observable A (without derivation)

$$\frac{d}{dt}A^H = \frac{1}{i\hbar}[A^H, H] \quad \text{with } A^H \equiv \mathcal{U}^\dagger A^S \mathcal{U}$$

G. Schrodinger's Wave Equation

- Examine $\Psi(x', t) = \langle x'|\alpha, t_0; t\rangle$
- Assume $H = p^2/2m + V(\mathbf{x})$
  - $\diamond$ $V(\mathbf{x})$ is an Hermitian operator
  - $\diamond$ $\langle x''|V(\mathbf{x})|x'\rangle = \delta(\mathbf{x}'' - \mathbf{x}')V(\mathbf{x}')$
- Recall

$$i\hbar\frac{\partial}{\partial t}|\alpha, t_0; t\rangle = H|\alpha, t_0; t\rangle$$

- Similarly

$$i\hbar\frac{\partial}{\partial t}\langle x'|\alpha, t_0; t\rangle = \langle x'|H|\alpha, t_0; t\rangle$$

- Therefore

$$i\hbar\frac{\partial}{\partial t}\langle x'|\alpha, t_0; t\rangle = \langle x'|\frac{-\nabla^2}{2m}|\alpha, t_0; t\rangle + \langle x'|V(\mathbf{x})|\alpha, t_0; t\rangle$$

- Apply ∇^2 and $V(\mathbf{x})$ to $\langle x'|$
- Altogether now

$$i\hbar\frac{\partial}{\partial t}\Psi(x', t) = \frac{-\hbar^2}{2m}\nabla^2\Psi(x', t) + V(x')\Psi(x', t) \tag{50}$$

  - $\diamond$ Starting point of wave mechanics
  - $\diamond$ Simple derivation from the Dirac formalism with the Hamiltonian as above
- Time-independent wave equation
  - $\diamond$ Identify $\Psi(x, t)$ as an energy eigenstate (stationary)
  - $\diamond$ For simplicity, replace $\Psi(x, t)$ with $u_E(x')$

$$u_E(x', t) = \mathrm{e}^{-iEt/\hbar}u_E(x')$$

◇ Insert into wave equation

$$\frac{-\hbar^2}{2m}\nabla'^2 u_E(x') + V(x')u_E(x') = E u_E(x') \tag{51}$$

V. Simple Harmonic Oscillator (SHO)

A. Energy eigenkets

- Hamiltonian → Motivated by classical mechanics

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 \tag{52}$$

  ◇ Let $k = m\omega^2$
  ◇ $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$

- Annihilation and Creation operators

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right)$$
$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right)$$

  ◇ Commuting $a, a^\dagger$

$$\begin{aligned}[a, a^\dagger] &= \frac{1}{2\hbar}\left(-i[x,p] + i[p,x]\right) \\ &= \frac{1}{2\hbar}(\hbar + \hbar) \\ &= 1\end{aligned}$$

- Number operator

$$\begin{aligned}N &= a^\dagger a \\ &= \frac{m\omega}{2\hbar}\left(x^2 + \frac{p^2}{m^2\omega^2}\right) + \frac{i}{2\hbar}[x,p] \\ &= \frac{H}{\hbar\omega} - \frac{1}{2}\end{aligned}$$

  ◇ $H = \hbar\omega(N + \frac{1}{2})$
  ◇ Clearly: $[N, H] = 0$

- Energy eigenkets

$$
\begin{aligned}
N|n\rangle &= n|n\rangle \\
H|n\rangle &= (n+\frac{1}{2})\hbar\omega|n\rangle
\end{aligned}
$$

  - ◇ Energies

$$E_n = (n+\frac{1}{2})\ \hbar\omega$$

- Restricting the values of n
  - ◇ Apply $a^\dagger, a$ to $|n\rangle$
  - ◇ Note

$$
\begin{aligned}
[N,a] &= [a^\dagger a, a] = a^\dagger[a,a] + [a^\dagger, a]a = -a \\
[N,a^\dagger] &= a^\dagger
\end{aligned}
$$

  - ◇ Therefore

$$
\begin{aligned}
Na^\dagger|n\rangle &= ([N,a^\dagger] + a^\dagger N)|n\rangle \\
&= (n+1)a^\dagger|n\rangle \\
Na|n\rangle &= (n-1)a|n\rangle
\end{aligned}
$$

  - ◇ $a^\dagger|n\rangle$ and $a|n\rangle$ are eigenstates of N with eigenvalues $n+1$ and $n-1$
  - ◇ Clearly

$$
\begin{aligned}
a|n\rangle &= c|n-1\rangle \\
\langle n|a^\dagger a|n\rangle &= n = |c|^2
\end{aligned}
$$

  - ◇ Therefore

$$
\begin{aligned}
a|n\rangle &= \sqrt{n}|n-1\rangle \\
a^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle
\end{aligned}
$$

  - ◇ Repeatedly applying a to $|n\rangle$

$$a^m|n\rangle = \sqrt{(n-1)(n-2)\ldots(n-m+1)}|n-m\rangle$$

  - ◇ If n is an integer, the series terminates at $n=0$ $\quad (a|0\rangle = 0)$
  - ◇ If n is non-integer, the series will not terminate

▲ But a contradiction appears!

$$<n|N|n> = n = \big(<n|a^\dagger\big) \cdot \big(a|n>\big) \geq 0$$

▲ Therefore $n \geq 0$ and n must exhibit the integer series

- Energies

$$E_n = (n + \frac{1}{2})\hbar\omega$$

  ◇ $n = 0, 1, 2, \ldots$

  ◇ Ground State

$$E_0 = \frac{1}{2}\hbar\omega$$

B. Position-wave functions

- Matrix elements for x, p

$$<n'|x|n> = \sqrt{\frac{\hbar}{2m\omega}} \big(\sqrt{n}\delta_{n',n-1} + \sqrt{n-1}\delta_{n',n+1}\big)$$
$$<n'|p|n> = i\sqrt{\frac{m\hbar\omega}{2}} \left(-\sqrt{n}\delta_{n',n-1} + \sqrt{n+1}\delta_{n',n+1}\right)$$

  ◇ Neither operator is 'diagonal' in the $\{|n>\}$ basis

  ◇ This was expected: $([x, H], [p, H] \neq 0)$

- Consider: $a|0> = 0$

  ◇ Position wave function

$$\begin{aligned} <x'|a|0> &= 0 \\ &= \sqrt{\frac{m\omega}{2\hbar}} <x'| \left(x + \frac{ip}{m\omega}\right) |0> \\ &= \sqrt{\frac{m\omega}{2\hbar}} \left[x'<x'|0> + \frac{i}{m\omega}<x'|p|0>\right] \end{aligned}$$

  ◇ Recall: $<x'|p|\alpha> = -i\hbar\frac{\partial}{\partial x'}<x'|\alpha>$

$$\left(x' + x_0^2\frac{d}{dx}\right)<x'|0> = 0 \quad \text{with} \quad x_0 \equiv \sqrt{\frac{\hbar}{m\omega}}$$

  ◇ Simple differential equation

◇ Solution for the ground state

$$<x'|0> = \frac{1}{(\pi x_0^2)^{1/4}} \exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right] \tag{53}$$

◇ Excited states are found trivially (creation operator)

$$\begin{aligned} <x'|1> &= <x'|a^\dagger|0> \\ &= <x'|\sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right)|0> \\ &= \frac{1}{\sqrt{2}x_0}\left(x' - x_0^2\frac{d}{dx'}\right)<x'|0> \end{aligned}$$

$$<x'|n> = \frac{1}{\pi^{1/4}\sqrt{2^n n!}}\left(\frac{1}{x_0^{n+\frac{1}{2}}}\right)\left(x' - x_0^2\frac{d}{dx}\right)^n \exp\left[-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right] \tag{54}$$

C. Expectation values

- Ground state

◇ x^2:

$$x^2 = \frac{\hbar}{2m\omega}(a^2 + a^{\dagger 2} + aa^\dagger + a^\dagger a)$$

$$\begin{aligned} < x^2 > &= <0|x^2|0> \\ &= \frac{\hbar}{2m\omega} = \frac{x_0^2}{2} \end{aligned}$$

◇ p^2:

$$< p^2 >= \frac{\hbar m\omega}{2}$$

▲ K.E.

$$< p^2/2m >= \frac{\hbar\omega}{4} = \frac{< H >}{2}$$

▲ P.E.

$$< m\omega^2 x^2/2 >= \frac{\hbar\omega}{4} = \frac{< H >}{2}$$

◇ $< x >=< p >= 0$ (as expected)

◇ Uncertainty relation

$$< (\Delta x)^2 > = < x^2 > = \frac{\hbar}{2m\omega}$$
$$< (\Delta p)^2 > = < p^2 > = \frac{\hbar m\omega}{2}$$
$$< (\Delta x)^2 >< (\Delta p)^2 > = \frac{\hbar^2}{4}$$

- Excited states

$$< (\Delta x)^2 >< (\Delta p)^2 > = \left(n + \frac{1}{2}\right)^2 \hbar^2$$

D. Time Evolution

- Schrodinger
  - ◇ Operators $x, p, a, a^\dagger$ are constant
  - ◇ Eigenstates evolve $|n(t)> = \mathcal{U}|n>$

$$|\alpha, t_0; t> = \sum_n c_n \mathrm{e}^{-i(n+\frac{1}{2})\omega t}|n>$$

- Heisenberg
  - ◇ State is constant
  - ◇ Operators evolve
- Operators: Equation of motion
  - ◇ p:

$$\begin{aligned}\frac{d}{dt}p &= \frac{1}{i\hbar}[p, H] = \frac{1}{i\hbar}[p, V(x)] \\ &= [p, m\omega^2 x^2/2] \\ &= \frac{m\omega^2}{2}\left(\,[p, x]x + x[p, x]\,\right) \\ &= -m\omega^2 x\end{aligned}$$

  - ◇ x:

$$\frac{d}{dt}x = \frac{p}{m}$$

  - ◇ $a, a^\dagger$:

$$\begin{aligned}&\frac{d}{dt}a = \frac{1}{i\hbar}[a, H] = -i\omega a \\ &\frac{d}{dt}a^\dagger = i\omega a^\dagger\end{aligned}$$

- Solutions
  - $\diamond$ $a, a^\dagger$

$$a(t) = a(0)\exp(-i\omega t)$$
$$a^\dagger(t) = a^\dagger(0)\exp(i\omega t)$$

  - $\diamond$ Express $a, a^\dagger$ in x, p

$$x(t) + \frac{ip(t)}{m\omega} = x(0)\exp(-i\omega t) + i\frac{p(0)}{m\omega}\exp(-i\omega t)$$
$$x(t) - \frac{ip(t)}{m\omega} = x(0)\exp(i\omega t) - i\frac{p(0)}{m\omega}\exp(i\omega t)$$

- Collecting real and imaginary terms

$$x(t) = x(0)\cos\omega t + \frac{p(0)}{m\omega}\sin\omega t$$
$$p(t) = -m\omega x(0)\sin\omega t + p(0)\cos\omega t$$

  - $\diamond$ These equations look like the classical equations of motion
  - $\diamond$ Similar oscillations as x, p in classical mechanics!
  - $\diamond$ 'Comfort' of the Heisenberg picture
  - $\diamond$ Do $< x >$ and $< p >$ oscillate with time?
  - $\diamond$ Not if $|\alpha>$ is an eigenstate of $|n>$

$$< x(t) > = < p(t) > = 0$$

  - $\diamond$ $< x >, < p >$ only oscillate for non-stationary states, e.g.

$$|\alpha> = c_0|0> + c_1|1>$$