

The Formalism of Quantum Mechanics

Our story so far...

- State of physical system: normalizable $\Psi(x, t)$
- Observables: operators \hat{x} , $\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$, \hat{H}
- Dynamics of Ψ : TDSE $i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi$

To solve, 1st solve TISE: $\hat{H} \Psi = E \Psi$

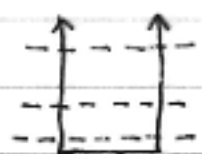
sol'ns are stationary states $\Psi_n(x)$, E_n

\Rightarrow special sol'ns of TDSE: $\Psi_n(x, t) = \Psi_n(x) e^{-iE_n t/\hbar}$

TDSE linear \Rightarrow any linear combo. of sol'n is also a solution

Discrete case: $\Psi(x, t) = \sum_n c_n e^{-iE_n t/\hbar} \Psi_n(x)$
 $(n = 1, 2, 3, \dots)$

Continuum case: $\Psi(x, t) = \int dk \phi(k) e^{-i\omega(k)t} \underbrace{\Psi_k(x)}_{e^{+ikx}/\sqrt{2\pi}}$
 $(k \text{ any real nbr})$



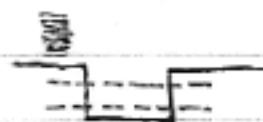
Discrete



Discrete



Continuum



Discrete +
Continuum

Ψ_n 's, Ψ_k 's form complete, orthonormal sets

$$\int dx \Psi_m^* \Psi_n = \delta_{mn}$$

$$\int dx \Psi_k^* \Psi_k = \frac{1}{2\pi} \int dx e^{i(k-k')x} = \delta(k-k')$$

Notice similarity of Ψ 's to vectors:

- Vector \vec{V} / complex fun $\Psi(x, t)$
- scalar real number a / complex nbr c
- any linear combination of vectors is a vector

$$\vec{C} = a\vec{A} + b\vec{B} \quad / \quad \Psi = \sum_n \alpha_n \Psi_n + \beta \Psi_i$$

- orthonormal basis vectors

$$\hat{x} \cdot \hat{x} = 1, \quad \hat{x} \cdot \hat{y} = 0 \quad / \quad \int \Psi_m^* \Psi_n dx = \delta_{mn}$$

$$\vec{V} = V_x \hat{x} + V_y \hat{y} + V_z \hat{z} \quad / \quad \Psi = \sum_n c_n \Psi_n$$

$$V_x = \hat{x} \cdot \vec{V} \quad / \quad c_n = \int dx \Psi_n^* \Psi$$

- inner product

$$\vec{A} \cdot \vec{B} = \sum_{i=x,y,z} A_i B_i \quad / \quad \int dx \Psi^* \Phi =$$

$$\int dx \left(\sum_m d_m \Psi_m \right)^* \left(\sum_n c_n \Psi_n \right)$$

$$= \sum_{m,n} d_m^* c_n \underbrace{\int \Psi_m^* \Psi_n dx}_{\delta_{mn}} = \sum_n d_n^* c_n$$

The space of all complex, square-integrable functions $\Psi(x)$ is called Hilbert Space

- Norm $\vec{V} \cdot \vec{V} = |\vec{V}|^2 \quad / \quad \int \Psi^* \Psi dx < \infty$

Hilbert Space is an infinite-dimensional ^{as a} vector space w/ complex scalars and normalizable vectors

Postulate 1: Every possible physical state of a system corresponds to a ^{normalized} vector in Hilbert Space. The correspondence is 1-to-1 except that vectors that differ by a phase factor (scalar of modulus 1) correspond to the same state $\Psi(x, t) \Leftrightarrow e^{i\theta} \Psi(x, t)$

Dirac Notation:

$$\int_{-\infty}^{+\infty} dx f^*(x) g(x) = \langle f | g \rangle = \text{complex nbr}$$

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

$\langle f | f \rangle$ is real, non-negative

$$c \text{ any complex nbr: } \langle f | c \cdot g \rangle = c \langle f | g \rangle$$

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

Postulate 2 (to be stated) associates w/ every observable a linear, hermitean operator.

Definition: An operator \hat{Q} is hermitean ~~is~~ if

$$\langle f | \hat{Q} g \rangle = \langle \hat{Q} f | g \rangle \text{ for all } f, g \text{ in Hilbert space (H-space)}$$

$$\int dx f^*(\hat{Q} g) = \int dx (\hat{Q} f)^* g$$

Is $\hat{Q} = \frac{d}{dx}()$ hermitean?

$$\underbrace{\int dx f^* dg/dx} \stackrel{?}{=} \int dx \left(\frac{df}{dx}\right)^* \cdot g$$

$$\text{parts: } \underbrace{f^*(x) g(x)}_0 \Big|_{-\infty}^{+\infty} - \int \frac{d}{dx}(f^*) \cdot g(x) dx = - \int \left(\frac{df}{dx}\right)^* \cdot g(x) dx$$

(No!)

Is $\hat{Q} = \frac{\hbar}{i} \frac{\partial}{\partial x}$ hermitean? Ans. Yes

$$\int f^* \frac{\hbar}{i} \frac{\partial g}{\partial x} dx \underset{\substack{\uparrow \\ \text{(parts)}}}{=} - \int \frac{\hbar}{i} \frac{d}{dx} (f^*) \cdot g = + \int \left(\frac{\hbar}{i} \frac{df}{dx} \right)^* g dx \quad \checkmark$$

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

Is $\hat{Q} = c \cdot ()$, $c = \text{constant}$ hermitean?

$$\langle f | c \cdot g \rangle \stackrel{?}{=} \langle c \cdot f | g \rangle$$

$$c \langle f | g \rangle \stackrel{?}{=} c^* \langle f | g \rangle \Rightarrow \text{hermitean only if } \underline{c \text{ real}}$$

Why are hermitean operators special? Why only hermitean operators associated w/ physical observables? Because hermitean operators produce real eigenvalues (and measurements of observables always produce real values).

$$\text{Eigenvalue equation: } \hat{Q} \underset{\substack{\uparrow \\ \text{eigenfunction}}}{f(x)} = \underset{\substack{\uparrow \\ \text{eigenvalue}}}{q} \cdot f(x)$$

Theorem: The eigenvalues of a hermitean operator \hat{Q} are real.

Proof: Assume $f(x) = \text{eigenfun}$: $\hat{Q} f = q f$

$$\langle Q \rangle \equiv \underbrace{\langle f | \hat{Q} f \rangle}_{q \langle f | f \rangle} \underset{\hat{Q} \text{ hermitean}}{=} \underbrace{\langle \hat{Q} f | f \rangle}_{\langle q \cdot f | f \rangle} = q^* \langle f | f \rangle$$

$$\Rightarrow (q - q^*) \langle f | f \rangle = 0 \Rightarrow q = q^* \quad (\text{since } \langle f | f \rangle \neq 0) \quad \checkmark$$

Theorem: The eigenfns of a hermitean operator w/ distinct (different) eigenvalues are orthogonal.

Proof: Given $\hat{Q} f(x) = q \cdot f(x)$, $\hat{Q} g(x) = q' \cdot g(x)$
w/ $q \neq q'$

$$\begin{aligned} \langle f | \hat{Q} g \rangle &= \langle \hat{Q} f | g \rangle \quad (\text{since } \hat{Q} \text{ hermitean}) \\ \underbrace{q'}_{\text{}} \langle f | g \rangle &= \underbrace{q^*}_{\text{(q real)}} \langle f | g \rangle = q \langle f | g \rangle \end{aligned}$$

$$\Rightarrow (q' - q) \langle f | g \rangle = 0 \Rightarrow \langle f | g \rangle = 0 \quad \text{since } (q' - q) \neq 0 \quad \checkmark \quad \text{by assumption}$$

Postulate 2 (Operator & Observables) This is a long postulate w/ 3 parts, and many texts break this up into 2 or 3 postulates

- 1) For every physical observable Q (x, p, E , etc) there corresponds a linear hermitean operator \hat{Q} in the Hilbert space which possesses a complete, orthonormal set of eigenfns $f_n(x)$ and corresponding eigenvalues q_n

$$\hat{Q} f_n(x) = q_n f_n(x) \quad (n \text{ could be discrete or continuous})$$

- 2) The only possible results of a measurement of Q are one of the eigenvalues $q_n = \{q_1, q_2, q_3, \dots\}$

- 3) The momentum operator is $\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x} ()$

The position operator is $\hat{x} = x \cdot ()$

Any function $Q(x, p)$ has operator $\hat{Q} = Q(\hat{x}, \hat{p})$

An example of $\hat{Q} = Q(\hat{x}, \hat{p})$:

energy operator $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} (\cdot) + V(x) \cdot (\cdot)$

Sol'ns of $\hat{H} \Psi_n = E_n \Psi_n$ form an orthonormal set (since \hat{H} is hermitean!). That Ψ_n 's form complete set can be proven in some special cases like infinite square well or S.H.O, but, in general, completeness is taken as a postulate.

If energy is measured, only possible results is one of the E_n 's.

The momentum eigenstates are sol'ns of:

$$\hat{p} f_p(x) = p \cdot f_p(x), \text{ where } \hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}.$$

Eigenfns: $f_p(x) = A e^{ikx}$ (any const A)

Eigenvalues: $p = \hbar k$ (k any real number)

Proof: $\frac{\hbar}{i} \frac{\partial}{\partial x} (A e^{ikx}) = \hbar k (A e^{ikx})$ ✓

In this case, the eigenvalues form a continuum (any real value of $p = \hbar k$ is permitted) and this leads to some mathematical subtleties.

Are the f_p 's orthonormal? (Ans: Kind of... yes)

$$\int f_{p'}(x) \cdot f_p(x) = \delta(p - p')$$

"Delta function orthogonality"