Review: Notation $\langle \hat{A} f | \hat{B} g \rangle = \int_a^b (\hat{A}f)^* (\hat{B}g)\, dx$

Observables correspond to **Hermitian Operators** $\hat{Q}$: $\langle \hat{Q} \rangle = \langle \hat{Q} \rangle^*$

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

$$\langle \hat{Q} h | h \rangle = \langle h | \hat{Q} h \rangle$$

Each hermitian $\hat{Q}$ generates a set of determinate states via $\underbrace{\hat{Q} f_q(x) = q f_q(x)}$ $\Rightarrow$ e.g. $\hat{H}\psi_n(x) = E_n \psi_n(x)$

f_q — eigenfunction (determinate state)

q — eigenvalue

$$\overbrace{\int_{-\infty}^{\infty} f_{p'}^*(x) f_p(x) dx}$$

For: $\hat{p} \Rightarrow f_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ip}{\hbar}x} \Rightarrow \overbrace{\langle f_{p'} | f_p \rangle} = \delta(p - p')$

$\hat{x} \Rightarrow g_y(x) = \delta(x - y) \Rightarrow \langle g_{y'} | g_y \rangle = \delta(y - y')$

} Dirac orthonormality

Using orthonormality we can express **any** $f(x)$ in Hilbert space as:

$$f(x) = \int_{-\infty}^{\infty} c(p) f_p(x) dp = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} c(p) e^{\frac{ipx}{\hbar}} dp$$

compare to:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, \psi(k,x,t)\, dk$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi^*(k,x,t)\, \Psi(x,t)\, dx$$

$$\boxed{c(p) = \int_{-\infty}^{\infty} f_p^*(x) f(x) dx} = \langle f_p | f \rangle$$

$$= \int_{-\infty}^{\infty} f_p^*(x) \left(\int_{-\infty}^{\infty} c(p') f_{p'}(x) dp' \right) dx$$

$$= \int_{-\infty}^{\infty} c(p') \Big[\underbrace{\int_{-\infty}^{\infty} f_p^*(x) f_{p'}(x) dx} \Big] dp'$$

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

$$= c(p)$$

$$f(x) = \int_{-\infty}^{\infty} c(y) g_y(x) dy = \int_{-\infty}^{\infty} c(y) \delta(y - x) dy$$

$$c(y) = \int_{-\infty}^{\infty} g_y^*(x) f(x) dx \equiv \langle g_y | f \rangle$$

$$= \int_{-\infty}^{\infty} g_y^*(x) \left(\int_{-\infty}^{\infty} c(y') g_{y'}(x) dy' \right) dx$$

$$= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} c(y') \delta(y - x) \delta(y' - x) dy' dx$$

$$= c(y)$$

Important point Since we can expand **any** $f(x)$, then each of these sets is a **complete** basis for the Hilbert space.

Having looked at the two "continuous" operators $\hat{x}, \hat{p}$ what about other $\hat{Q}$? We find continuous, discrete, both

treat one at a time

Things we can say about "discrete" $\hat{Q}$s,

a) Eigenvalues are real (actually obvious since $\langle \hat{Q} \rangle = \langle \hat{Q} \rangle^*$)

$\langle h | \hat{Q} h \rangle = \langle \hat{Q} h | h \rangle$ take $\hat{Q} h = q_h h$

$\langle h | q_h h \rangle = \langle q_h h | h \rangle$

$q_h \cancel{\langle h | h \rangle}^{1} = q_h^* \cancel{\langle h | h \rangle}^{1}$

$q_h = q_h^* \Rightarrow q_h$ is real

b) Determinant states (eigenstates) of $\hat{Q}$ are orthogonal.

$\langle f | \hat{Q} g \rangle = \langle \hat{Q} f | g \rangle$ take $\hat{Q} g = q_g g$, $\hat{Q} f = q_f f$

$\langle f | q_g g \rangle = \langle q_f f | g \rangle$ assume $q_g \neq q_f$

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

$q_f^* = q_f \neq q_g \Rightarrow \boxed{\langle f | g \rangle = 0}$

c) The determinate states form a complete set.

Moral: Each hermitian operator $\hat{Q}$ corresponding to an observable generates a complete orthonormal basis in Hilbert space from its eigen vectors (determinant states).

Our goal has been $\Psi(x,t)$ from TDSE.
But we know $\Psi(x,t)$ lives in Hilbert space.
Each hermitian operator generates an orthonormal basis of Hilbert space.

$\Rightarrow$ $\Psi(x,t)$ can be decomposed into the determinant states of any $\hat{Q}$.

$$\boxed{\Psi(x,t) = \sum_n \overbrace{c_n}^{c_n(t)} \underbrace{f_n(x)}_{\text{determinant states of } \hat{Q}}}$$

where $\boxed{c_n = \int f_n^*(x)\, \Psi(x,t)\, dx \equiv \langle f_n | \Psi \rangle}$

The program:

i) Get Ψ from TDSE

ii) Pick what you want to measure (energy, position, $\vec{p}$)

iii) Form the hermitian operator ($\hat{H}, \hat{x}, \hat{p}$)

iv) Expand Ψ in the appropriate basis of $\hat{Q}$.

v) Expansion coefficients c_n give the probabilities $|c_n|^2$ of each result.

vi) Expectation values follow: $\langle \hat{Q} \rangle = \sum_n |c_n|^2 q_n$
where q_n comes from $\hat{Q} f_n(x) = q_n f_n(x)$.