

Similar to the spatial translation operator $T(\Delta x)|x\rangle = |x + \Delta x\rangle$
(unitary)

We can construct a unitary operator for time evolution:

$$U(t, t_0) |\psi; t_0\rangle = |\psi; t\rangle$$

note: $|\psi; t_0\rangle = \sum_i c_i(t_0) |i\rangle$

→ some eigenbasis $\{|i\rangle\}$

e.g., $\{|x\rangle\}$ or $\{|p\rangle\}$

and $|\psi; t\rangle = \sum_i c_i(t) |i\rangle$

$c_i(t) \neq c_i(t_0)$

we did not time evolve the eigenbasis $\{|i\rangle\}$.

[we could have, but we choose not to]

the operator for an infinitesimal time step dt of time evolution is

$$U(t_0 + dt, t_0) = \mathbb{1} - i \frac{dt}{\hbar} H$$

H = Hamiltonian for the system

We can now look at ^{the} time evolution of $U(t, t_0)$:

$$U(t+dt, t_0) = U(t+dt, t) U(t, t_0) = \left(\mathbb{1} - i \frac{dt}{\hbar} H \right) U(t, t_0)$$

$t - t_0$ is not infinitesimal

$$= U(t, t_0) - \frac{i dt}{\hbar} H U(t, t_0)$$

$$\Rightarrow \frac{U(t+dt, t_0) - U(t, t_0)}{dt} = -\frac{i}{\hbar} H U(t, t_0)$$

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

Schrodinger equation for the time evolution operator $U(t, t_0)$.

Multiply
on the
right by
a ket
 $|\psi; t_0\rangle$

$$i\hbar \frac{\partial}{\partial t} \underbrace{U(t, t_0) |\psi; t_0\rangle}_{|\psi; t_0 \rightarrow t\rangle} = H \underbrace{U(t, t_0) |\psi; t_0\rangle}_{|\psi; t_0 \rightarrow t\rangle}$$

$$\Rightarrow i\hbar \frac{\partial}{\partial t} \underbrace{|\psi; t_0 \rightarrow t\rangle}_{|\psi(t)\rangle} = H \underbrace{|\psi; t_0 \rightarrow t\rangle}_{|\psi(t)\rangle}$$

Schrodinger equation for the ket $|\psi; t_0\rangle$

In the case of a time-independent Hamiltonian H , then

$$U(t, t_0) = \exp\left[-\frac{i}{\hbar} H (t - t_0)\right] = \exp\left[-\frac{i(t-t_0)}{\hbar} H\right]$$

H is an operator

$$= \lim_{N \rightarrow \infty} \left[1 - \frac{i}{\hbar} \frac{H (t - t_0)}{N} \right]^N$$

$$= 1 + \left(\frac{-i(t-t_0)}{\hbar} \right) H + \frac{1}{2!} \left(\frac{-i(t-t_0)}{\hbar} \right)^2 H^2 + \frac{1}{3!} \left(\frac{-i(t-t_0)}{\hbar} \right)^3 H^3 + \dots$$

! Calculating $\exp\left[-\frac{i(t-t_0)}{\hbar} H\right]$ is very difficult, unless you go the eigenbasis of H ... then it's relatively easy.

recall:
 $e^A = \sum_{n=0}^{\infty} \frac{1}{n!} A^n$
note: $A^0 = \mathbb{1}$

The eigenstates of the Hamiltonian operator simplify these equations / expressions significantly:

$$H|\psi_E\rangle = E|\psi_E\rangle$$

↑ Hermitian
 ↑ Eigenvalue = Eigen energy ($E \in \mathbb{R}$)
 eigenstate = stationary state

time evolution: $U(t, t_0)|\psi_E\rangle = e^{-i\frac{(t-t_0)}{\hbar}H}|\psi_E\rangle$ ← potentially hard to calculate

Energy eigenstates [i.e., stationary states] do not change in time, except for an overall phase factor

$$= e^{-i\frac{(t-t_0)}{\hbar}E}|\psi_E\rangle$$

← easy to calculate

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

Likewise, the Schrodinger equation is simple to solve with the ~~the~~ energy eigenstates:

$$i\hbar \frac{\partial}{\partial t} |\psi_E(t)\rangle = H|\psi_E(t)\rangle = E|\psi_E(t)\rangle$$

$$\Rightarrow |\psi_E(t)\rangle = e^{-i\frac{(t-t_0)}{\hbar}E} |\psi(t_0)\rangle$$

Note: Figuring out ~~the~~ (i.e., determining) the energy eigenstate is not-so-easy.

Once the energy eigenbasis is determined $\{|\psi_{E_n}\rangle\}$, then the time evolution for any state can be easily determined:

If $|\psi(t=0)\rangle = \sum_n C_n |\psi_{E_n}\rangle$

$$\Rightarrow \text{then } |\psi(t)\rangle = \sum_n C_n e^{-i\frac{E_n t}{\hbar}} |\psi_{E_n}\rangle$$

$C_n(t)$

"Good Quantum Number"

Consider an operator A (with eigenstates $\{|a_i\rangle\}$) that commutes and eigenvalues $\{a_i\}$

with H : $[H, A] = 0$ and $A|a_i\rangle = a_i|a_i\rangle$

then the time evolution of the $|a_i\rangle$ eigenstates is simple

If $|a_i(t)\rangle = U(t) \underbrace{|a_i\rangle}_{|a_i(t=0)\rangle}$, then we can calculate $A|a_i(t)\rangle$

$$A|a_i(t)\rangle = A e^{-iHt/\hbar} |a_i\rangle = e^{-iHt/\hbar} \underbrace{A|a_i\rangle}_{a_i|a_i\rangle} = a_i e^{-iHt/\hbar} |a_i\rangle$$

$[H, A] = 0$

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

$\Rightarrow |a_i(t)\rangle$ remains an eigenstate of $A \Rightarrow a_i$ is a "good quantum number"

Note: $|a_i\rangle$ is also an eigenstate of H .

Schrodinger Wave Equation

The Hamiltonian for a single particle ^(of mass m) moving in an external potential $V(x)$ [$V(x)$ = potential energy] is

$$H = \frac{P^2}{2m} + V(x) = \frac{1}{2m} P^2 + V(x)$$

$\uparrow$ P operator $\uparrow$ x operator

The Schrodinger equation becomes

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

In position space (x -representation / basis), we get

$$\langle x | i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \langle x | H |\psi(t)\rangle$$

$$\begin{aligned} \Rightarrow i\hbar \frac{\partial}{\partial t} \underbrace{\langle x | \psi(t) \rangle}_{\psi(x,t)} &= \underbrace{\langle x | \frac{1}{2m} P^2 |\psi(t)\rangle}_{\frac{1}{2m} \langle x | P \cdot P |\psi(t)\rangle} + \underbrace{\langle x | V(x) |\psi(t)\rangle}_{= \langle x | V(x) \uparrow_{\text{scalar } x} \psi(t) = V(x) \langle x | \psi(t) \rangle} \\ &\quad \begin{array}{l} \text{operator } x \\ \text{scalar } x \end{array} \end{aligned}$$

$$-i\hbar \int dx'' \langle x'' | x' \rangle \frac{\partial}{\partial x''} \langle x'' |$$

$$\frac{-\hbar^2}{2m} \left(\int dx'' \underbrace{\langle x | x'' \rangle}_{\delta(x-x'')} \frac{\partial}{\partial x''} \underbrace{\langle x'' |}_{\langle x'' | x' \rangle = \delta(x''-x')} \int dx' \langle x' | \frac{\partial}{\partial x'} \langle x' | \psi(t) \rangle \right)$$

$$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t)$$

$$\Rightarrow i\hbar \frac{\partial}{\partial t} \psi(x,t) = \underbrace{\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x,t)}_{H} + V(x) \psi(x,t)$$

$$= \left[\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] \psi(x,t)$$

Schrodinger Wave Equation

This equation is much easier to solve, if we look for the stationary state ~~st~~ solutions: $\Psi_E(x,t) = e^{-\frac{iEt}{\hbar}} \psi_E(x)$

Where $\left\{ \begin{matrix} \psi_E(x) \\ E \end{matrix} \right\}$ satisfies:
$$\underbrace{\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right]}_{\text{"H"}} \psi_E(x) = E \psi_E(x)$$

Note 1: We require that $\int_{-\infty}^{+\infty} \psi_E^*(x) \psi_E(x) dx = 1$ Eigenenergy - eigenstate equation to be normalized for a continuous eigenbasis

Note 2: $\{|\psi_{E_n}\rangle\}$ form an eigenbasis: $\sum_n |\psi_{E_n}\rangle \langle \psi_{E_n}| = 1$

or $\int dn |\psi_{E_n}\rangle \langle \psi_{E_n}| = 1$

orthonormality: $\langle \psi_{E_n} | \psi_{E_{n'}} \rangle = \begin{cases} \delta_{nn'} & \text{discrete} \\ \delta(n-n') & \text{continuous} \end{cases}$

Heisenberg "Picture" of time evolution

Schrodinger picture: $\begin{cases} \text{Operator/observable are time-independent} \\ \text{kets evolve in time} \end{cases}$

Heisenberg picture: $\begin{cases} \text{Operators evolve in time} \\ \text{kets are time independent} \end{cases}$

Consider $\langle \psi_1(t) | A | \psi_2(t) \rangle = \langle \psi_1 | e^{\frac{iHt}{\hbar}} A e^{-\frac{iHt}{\hbar}} | \psi_2 \rangle$

In the Heisenberg picture $A \rightarrow A(t) = e^{\frac{iHt}{\hbar}} A e^{-\frac{iHt}{\hbar}}$