Schrödinger equation & free particle

Postulate 4: Evolution of state

Evolution of states is governed by

Classical	Quantum
$x(t_0), p(t_0) \longrightarrow x(t), p(t)$ Hamilton's (canonical) equations $\dfrac{dx(t)}{dt} = \dfrac{\partial H}{\partial p}, \qquad \dfrac{dp(t)}{dt} = -\dfrac{\partial H}{\partial x}$	$\lvert\psi(t_0)\rangle \longrightarrow \lvert\psi(t)\rangle$ Schrödinger equation $i\hbar \dfrac{d}{dt}\lvert\psi(t)\rangle = \hat{H}\lvert\psi(t)\rangle$ $\hat{H}(\hat{X}, \hat{P}) = H(x \to \hat{X}, p \to \hat{P})$ Hamiltonian operator

P4: Evolution of states

How to solve $i\hbar \frac{d}{dt}\left|\psi(t)\right\rangle = \hat{H}\left|\psi(t)\right\rangle$

Solve first $\hat{H}|E\rangle = E|E\rangle$ Time-independent Schrödinger equation

Insert $|\psi(t)\rangle = \sum_i |E_i\rangle\langle E_i|\psi(t)\rangle$ into the S. E. $\longrightarrow$ $\langle E_i|\psi(t)\rangle = \langle E_i|\psi(0)\rangle \exp\left(-\frac{iE_i t}{\hbar}\right)$

$$\therefore |\psi(t)\rangle = \sum_i |E_i\rangle\langle E_i|\psi(0)\rangle \exp\left(-\frac{iE_i t}{\hbar}\right)$$

(Question) How will the state $|\psi(0)\rangle = \frac{1}{\sqrt{2}}[|E_1\rangle + |E_2\rangle]$ evolve with time?

(1) Eigenstates of $\hat{H}$ are stationary states.

$$|E_j(t)\rangle = \sum_i |E_i\rangle\langle E_i|E_j\rangle \exp\left(-\frac{iE_i t}{\hbar}\right) = |E_j\rangle \exp\left(-\frac{iE_j t}{\hbar}\right)$$

For any observable $\hat{\Omega}$, the probability distribution is time-independent.

$$P(\omega, t) = \left|\left\langle \omega \middle| E_j(t)\right\rangle\right|^2 = \left|\left\langle \omega \middle| E_j(0)\right\rangle\right|^2 = P(\omega, 0)$$

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$$\therefore |\psi(t)\rangle = \sum_i |E_i\rangle\langle E_i|\psi(0)\rangle \exp\left(-\frac{iE_i t}{\hbar}\right)$$

(2) Propagator $\hat{U}$

$$|\psi(t)\rangle = \hat{U}(t,0)|\psi(0)\rangle$$

$$\hat{U}(t,0) = \sum_i |E_i\rangle\langle E_i| \exp\left(-\frac{iE_i t}{\hbar}\right)$$

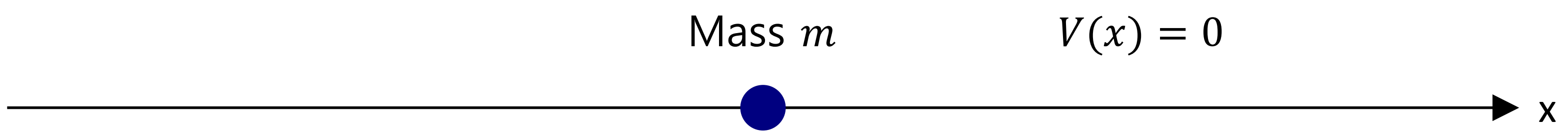
$$\hat{U}(t_2,t_1) = \sum_i |E_i\rangle\langle E_i| \exp\left(-\frac{iE_i(t_2-t_1)}{\hbar}\right)$$

$$|\psi(t_1)\rangle \xrightarrow{\hat{U}(t_2,t_1)} |\psi(t_2)\rangle \xrightarrow{\hat{U}(t_3,t_2)} |\psi(t_3)\rangle \longrightarrow \cdots$$

$$\hat{U}(t_3,t_1) = \hat{U}(t_3,t_2)\hat{U}(t_2,t_1)$$

$$\hat{U}(t_1,t_2) = \underbrace{\hat{U}^\dagger(t_2,t_1) = \hat{U}^{-1}(t_2,t_1)}_{\text{Unitary operator}}$$

(Ex1) Free particle



$H = \dfrac{p^2}{2m}$ (Classical) Hamiltonian $\qquad$ $\hat{H} = \dfrac{\hat{P}^2}{2m}$ (Quantum) Hamiltonian operator

$\hat{H}|E\rangle = \dfrac{\hat{P}^2}{2m}|E\rangle = E|E\rangle$ Time-independent Schrödinger equation

$[\hat{H}, \hat{P}] = 0$ $\qquad$ $\hat{H}$ and $\hat{P}$ have simultaneous eigenstates.
Any momentum eigenstate $|p\rangle$ is also an eigenstate of $\hat{H}$.

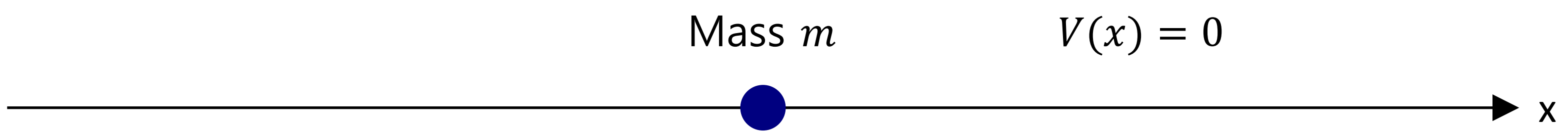
$E = \dfrac{p^2}{2m}$

$p = \pm\sqrt{2mE}$

- Eigenvalue E is continuous.
- For each eigenvalue E, there are two degenerate eigenstates.
  $|E,+\rangle = |p = +\sqrt{2mE}\rangle, \quad |E,-\rangle = |p = -\sqrt{2mE}\rangle$
- $|E\rangle = \alpha_+|E,+\rangle + \alpha_-|E,-\rangle$ is also an eigenstate of $\hat{H}$ with eigenvalue E.
  (But, it is not in general an eigenstate of $\hat{P}$.)
- In the X basis, $\psi_E(x) = \langle x|E\rangle = \alpha_+\underline{\langle x|E,+\rangle} + \alpha_-\underline{\langle x|E,-\rangle}$

Do you remember what these are?

(Ex1) Free particle



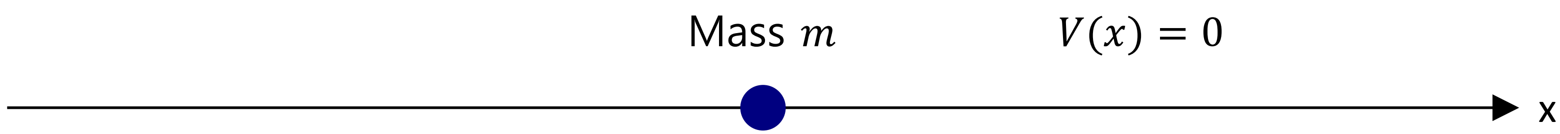
$$|\psi(t)\rangle = \hat{U}(t,0)|\psi(0)\rangle$$

$$\psi(x,t) = \langle x|\psi(t)\rangle = \langle x|\hat{U}(t,0)|\psi(0)\rangle = \int_{-\infty}^{\infty} \langle x|\hat{U}(t,0)|x'\rangle \underbrace{\langle x'|\psi(0)\rangle}_{\psi(x',0)} dx'$$

$$\hat{U}(t,0) = \sum_i |E_i\rangle\langle E_i| \exp\left(-\frac{iE_i t}{\hbar}\right) \longrightarrow \hat{U}(t,0) = \int_{-\infty}^{\infty} |p\rangle\langle p| \exp\left(-\frac{ip^2 t}{2m\hbar}\right) dp$$

$$\langle x|\hat{U}(t,0)|x'\rangle = \int_{-\infty}^{\infty} \langle x|p\rangle\langle p|x'\rangle \exp\left(-\frac{ip^2 t}{2m\hbar}\right) dp = \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left(\frac{im(x-x')^2}{2\hbar t}\right)$$

(Ex1) Free particle



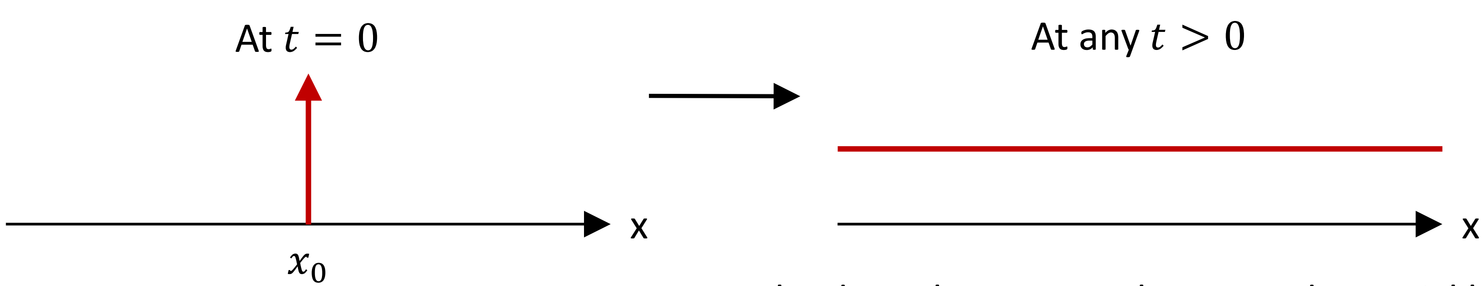
$$\psi(x,t) = \int_{-\infty}^{\infty} \underline{\langle x|\widehat{U}(t,0)|x'\rangle}\psi(x',0)dx'$$

$$\langle x|\widehat{U}(t,0)|x'\rangle = \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left(\frac{im(x-x')^2}{2\hbar t}\right)$$

(Case 1) Particle localized at $x = x_0$ at $t = 0$

$$\psi(x',0) = \langle x'|x_0\rangle = \delta(x' - x_0)$$

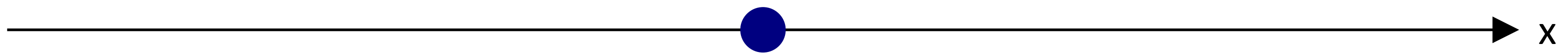
$$\therefore\ \psi(x,t) = \langle x|\widehat{U}(t,0)|x_0\rangle$$ Propagator itself



Why does the wavepacket spread so quickly?

(Ex1) Free particle

Mass m $\qquad$ $V(x) = 0$



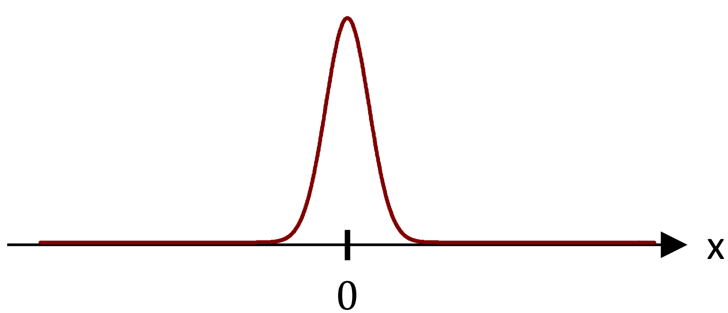
$$\psi(x,t) = \int_{-\infty}^{\infty} \langle x|\hat{U}(t,0)|x'\rangle \psi(x',0)dx'$$

$$\langle x|\hat{U}(t,0)|x'\rangle = \sqrt{\frac{m}{2\pi i\hbar t}} \exp\left(\frac{im(x-x')^2}{2\hbar t}\right)$$

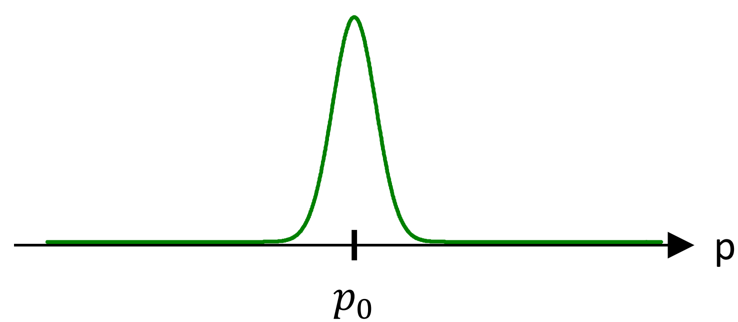
(Case 2) Gaussian wavepacket centered at $x = 0$ with a mean momentum p_0 at $t = 0$

$$\psi(x) = \frac{1}{(\pi\Delta)^{1/4}} e^{ip_0 x} e^{-x^2/2\Delta^2}$$

$\langle X\rangle = 0,\ \Delta X = \Delta/\sqrt{2}$

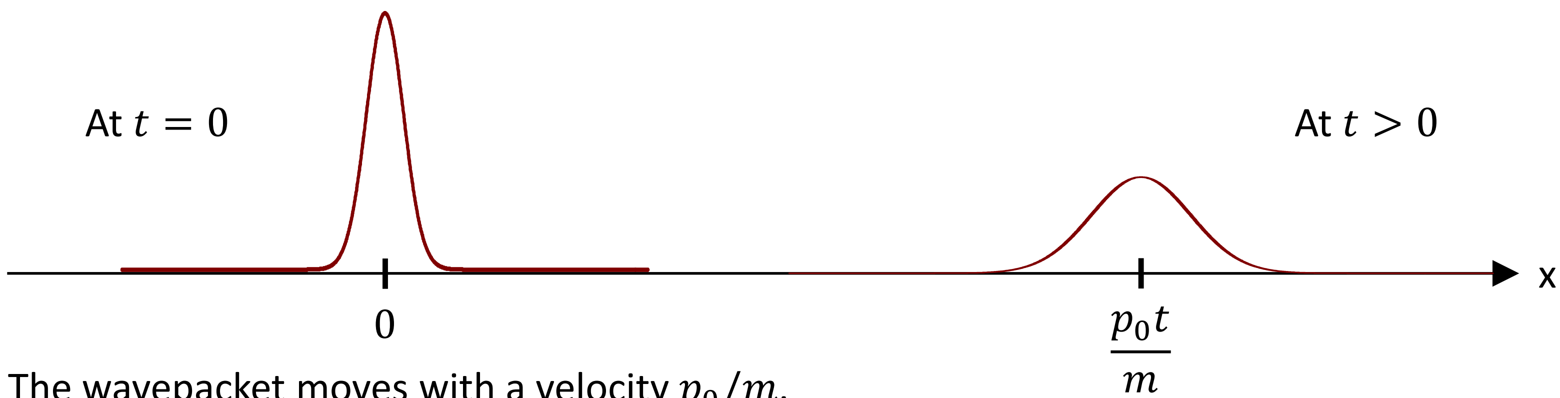


$\langle P\rangle = p_0,\ \Delta P = \hbar/\sqrt{2}\Delta$



(Ex1) Free particle

Results of tedious arithmetic (you should to it)



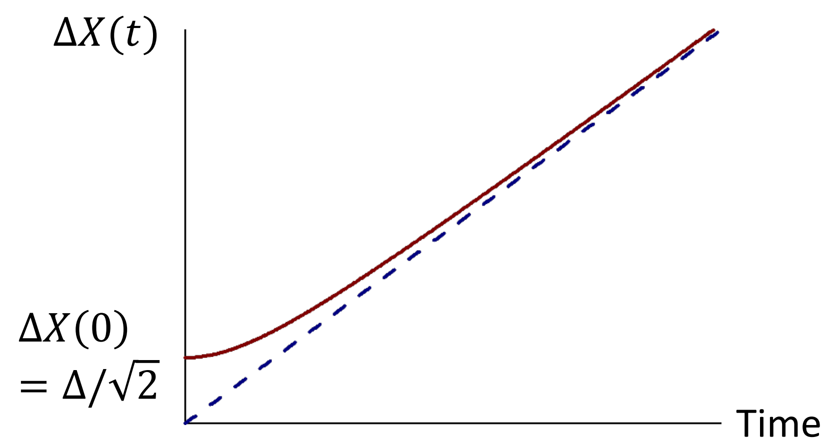
(1) The wavepacket moves with a velocity p_0/m.

Quantum

Classical

$$\langle X \rangle = \frac{p_0 t}{m} = \frac{\langle P \rangle t}{m} \longleftrightarrow x = \frac{pt}{m}$$

Ehrenfest's theorem



(2) The wavepacket spreads with time.

$$\Delta X(t) = \Delta X(0)\sqrt{1 + \left(\frac{\hbar t}{m\Delta^2}\right)^2}$$

- Why does the wavepacket spread with time?
- Can you pre-estimate the slope of the blue dashed line based on the Heisenberg uncertainty principle?