# Back to Wave Mechanics: Continuum States and Scattering

Consider a single spinless particle in $d = 1, 2,$ or $3$ spatial dimensions.

$$i\hbar \frac{d}{dt}|\psi\rangle = \hat{H}(t)|\psi\rangle \;;\quad \hat{H}(t) = \frac{\hat{\vec{P}}^2}{2m} + \hat{V}(\hat{\vec{x}}, t)$$

- Allows time-dept. external force, e.g. electric field $\vec{E}(\vec{x},t)$
- $\vec{E}(\vec{x},t) = -\frac{1}{c}\partial_t \vec{A} - \vec{\nabla} V$
  $\vec{B}(\vec{x},t) = \vec{\nabla}\times\vec{A}$
  "Vector Potential"
  - Needed to couple motion of (spinless) quantum particle to a magnetic field $\vec{B}(\vec{x},t)$
  - Excluded for now.

Electric $\vec{E}$, magnetic $\vec{B}$ fields in terms of "gauge potentials"

## 1. Probability Current

Conservation Law $\Rightarrow$ Continuity Equation

- Consider a classical fluid consisting of particles that cannot be created or destroyed — Total particle number $\equiv N$ is conserved. e.g., • Liquid water ($H_2O$ molecules)
  • 1-component plasma ($e^-$ in ionosphere)

Let $\rho(\vec{x},t) \equiv$ particle number density $\quad (1/L^d)$

$\vec{J}(\vec{x},t) \equiv$ particle number current density; $\left(\frac{L}{t}\right) \times \left(\frac{1}{L^d}\right)$

Flux or Velocity; Density

Regardless of the dynamics

(Forces acting, distribution of particle velocities, etc.), these must satisfy the

**Continuity Equation:** $\quad \partial_t \rho + \vec{\nabla}\cdot\vec{J} = 0.$

To see why, integrate this equation over the volume:

$$\int d^d\vec{x}\; \partial_t \rho(\vec{x},t) = \frac{d}{dt}\int d^d\vec{x}\; \rho(\vec{x},t) = \frac{dN}{dt} = -\int d^d\vec{x}\; \vec{\nabla}\cdot\vec{J} \underset{\text{Divergence Theorem}}{=} -\underbrace{\oint_S d^{d-1}\vec{x}\; \hat{n}\cdot\vec{J}}_{\text{Integral over boundary surface}} = -\begin{pmatrix}\text{Particle} \\ \text{flux} \\ \text{leaving} \\ \text{volume}\end{pmatrix}$$

$\therefore \dfrac{dN}{dt} = 0$ if no particle flux through system boundary.

## What is Conserved in Single-Particle Quantum Mechanics?

**Probability.** (At least, in between projective measurements)

- $\rho(\vec{x},t) \equiv |\psi(\vec{x},t)|^2$, probability density to find particle at $\vec{x}$, at time $t$; $\int d^d\vec{x}\; \rho(\vec{x},t) = 1$

$$\partial_t \rho = \dot{\psi}^*\psi + \psi^*\dot{\psi} \;;\quad \dot{\psi}(\vec{x},t) = \frac{-i}{\hbar}\left[\frac{-\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{x},t)\right]\psi(\vec{x},t)$$

$$\dot{\psi}^*(\vec{x},t) = \frac{i}{\hbar}\left[\frac{-\hbar^2}{2m}\vec{\nabla}^2 + V(\vec{x},t)\right]\psi^*(\vec{x},t)$$

$$\Rightarrow \partial_t P = \frac{i}{\hbar}\left[-\frac{\hbar^2}{2m}(\nabla^2\psi^*)\psi + \frac{\hbar^2}{2m}\psi^*\nabla^2\psi\right]$$

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Let us define

Imaginary Part

$$\vec{J} \equiv \frac{\hbar}{2mi}\left[\psi^*\vec{\nabla}\psi - (\vec{\nabla}\psi^*)\psi\right] \equiv \frac{\hbar}{2mi}\left(\psi^*\overleftrightarrow{\nabla}\psi\right) = \frac{\hbar}{m}\,\mathrm{Im}\left[\psi^*\vec{\nabla}\psi\right]$$

"Double-sided derivative": $A\overleftrightarrow{\nabla}B \equiv A\vec{\nabla}B - (\vec{\nabla}A)B$

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$$\vec{\nabla}\cdot\vec{J} = \frac{\hbar}{2mi}\left[\cancel{\vec{\nabla}\psi^*\cdot\vec{\nabla}\psi} + \psi^*\nabla^2\psi - (\nabla^2\psi^*)\psi - \cancel{\vec{\nabla}\psi^*\cdot\vec{\nabla}\psi}\right] = -\partial_t P \checkmark$$

$\therefore$ $\vec{J}$ defined above is the Probability Current Density

$\Rightarrow$ Describes the flow (magnitude and direction) of probability in space and time.

1D version: $\partial_t P + \partial_x J = 0$; $P = |\psi|^2$; $J = \frac{\hbar}{m}\,\mathrm{Im}\left[\psi^*\partial_x\psi\right]$ Probability Current (units 1/time)

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## ② Free Particle in 1D; Gaussian Wavepacket

$\hat{H} = \frac{\hat{p}^2}{2m}$ ; $\hat{H}|p\rangle = E_p|p\rangle$, $E_p = \frac{p^2}{2m}$ Momentum Basis = Energy Eigenbasis

[Note: $|p\rangle$ and $|-p\rangle$ are "degenerate": share same energy eigenvalue.]

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{ipx}{\hbar}} \equiv \psi_p(x)$$

Time Evolution: $\langle x|\hat{U}(t)|p\rangle \equiv \psi_p(x,t) = \langle x|e^{\frac{-i\hat{H}t}{\hbar}}|p\rangle = \underbrace{e^{\frac{-iE_pt}{\hbar}}}_{\text{Pure Phase}}\psi_p(x)$

Pure Phase (As always, for energy eigenstate)

- Probability Density:

$P_p(x) \equiv |\psi_p(x,t)|^2 = \frac{1}{2\pi\hbar}$, uniform in space (and non-normalizable: $\langle p|p'\rangle = \delta(p-p')$ )

- Probability Current: $\psi_p^*\frac{d}{dx}\psi_p = \frac{1}{2\pi\hbar}\frac{ip}{\hbar} \Rightarrow J = \frac{\cancel{\hbar}}{m}\frac{1}{2\pi\hbar}\frac{p}{\cancel{\hbar}} = P\times\frac{p}{m} = \underbrace{|\psi_p(x)|^2}_{\text{Prob. Density}}\times\underbrace{\left(\frac{p}{m}\right)}_{\text{Velocity!}}$

$\therefore$ Although $|p\rangle$ and $|-p\rangle$ both share energy $E_p = \frac{p^2}{2m}$,

$|p\rangle$ ($|-p\rangle$) describes a probability flux to the right (left), respectively ($p>0$)

$\Rightarrow \langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{ipx}{\hbar}}$ : $\longrightarrow$ RIGHT-MOVING FLUX

$\langle x|-p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{-ipx}{\hbar}}$ : $\longleftarrow$ LEFT-MOVING FLUX

($p>0$)

# TIME EVOLUTION FOR A GENERAL INITIAL STATE: THE PROPAGATOR

$$|\psi(t)\rangle = \hat{U}(t)\,|\psi_0\rangle\,;\quad \hat{U}(t) = e^{-i\frac{\hat{H}t}{\hbar}}\int_{-\infty}^{\infty} dp\, |p\rangle\langle p| = \int_{-\infty}^{\infty} dp\, |p\rangle\langle p|\, e^{-i\frac{p^2}{2m\hbar}t}$$

POSITION BASIS REPRESENTATION: $\langle x|\hat{U}(t)|x'\rangle \equiv U(x,x';t) = \int_{-\infty}^{\infty}\frac{dp}{2\pi\hbar}\, e^{\frac{ip(x-x')}{\hbar}}\, e^{-\frac{1}{2}\left(\frac{it}{m\hbar}\right)p^2}$

↑ POSITION BASIS "PROPAGATOR"; OFTEN, JUST "THE PROPAGATOR"

GAUSSIAN INTEGRAL: LEC 9, p. 2

$$\int_{-\infty}^{\infty} dy\, e^{-\frac{\alpha y^2}{2}+\beta y} = \left(\frac{2\pi}{\alpha}\right)^{\frac{1}{2}} e^{\frac{\beta^2}{2\alpha}} \qquad (1)$$

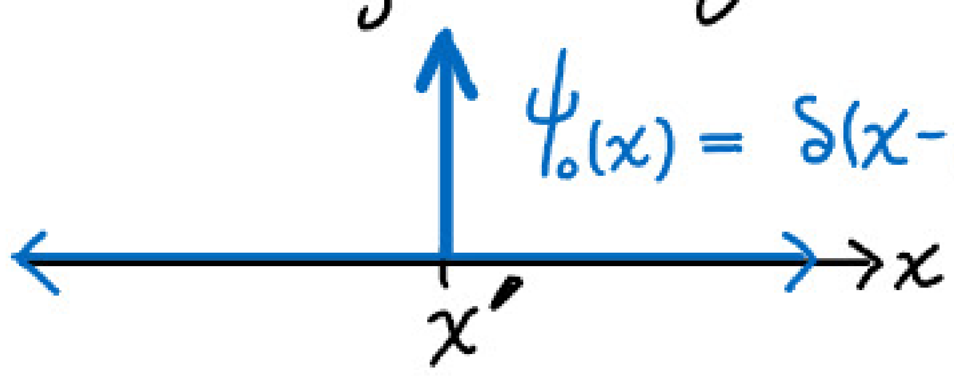
- $\alpha = \frac{it}{m\hbar}$ (PURELY IMAGINARY! → CLAIM: OK TO STILL USE Eq. (1) BECAUSE RAPID OSC. AS $|p|\to\infty$ GIVES CONVERGENCE)
- $\beta = \frac{i(x-x')}{\hbar}$ (ALSO PURE IMAG.)

$$\Rightarrow\quad U(x,x';t) = \left(\frac{2\pi}{it/m\hbar}\right)^{\frac{1}{2}}\frac{1}{2\pi\hbar}\, e^{-\frac{m\hbar}{2it}\frac{(x-x')^2}{\hbar^2}} = \left(\frac{m}{2\pi i\hbar t}\right)^{\frac{1}{2}} e^{\frac{im(x-x')^2}{2\hbar t}}$$

UNITS: $[m] = \text{ENERGY}\left(\frac{\text{TIME}}{\text{LENGTH}}\right)^2 \Rightarrow \left[\frac{mx^2}{\hbar t}\right] = \frac{\text{ENERGY}\cdot\text{TIME}^2}{\text{ENERGY}\cdot\text{TIME}^2}$ = DIM.LESS ✓

## WHAT IS $U(x,x';t)$? ("THE PROPAGATOR")

① PROBABILITY AMPLITUDE TO EVOLVE FROM δ-FUNCTION LOCALIZED INITIAL POSITION:




$\psi_0(x) = \delta(x-x')$ ; $\psi(x,t) = U(x,x';t)$

$$|U(x,x';t)|^2 = \left(\frac{m}{2\pi\hbar t}\right),$$ INDEPT. OF $x, x'$ FOR ANY $t\neq 0$.

⇒ SPREADS INFINITELY FAST! ? CAUSALITY ?

WHY? FOR $|\psi_0\rangle = |x'\rangle$, $\Delta X = 0 \Rightarrow \Delta P \geq \frac{\hbar}{2\Delta X} \to \infty$

∴ STARTING FROM A POSITION EIGENKET (δ-FUNCTION IN $x$) MEANS A SUPERPOSITION OF ALL MOMENTA.

- NON-RELATIVISTIC Q.M.: INITIAL STATE CONTAINS MOMENTUM WAVES WITH ARBITRARILY LARGE (PHASE) VELOCITY $P/m \to \infty$

∴ INCONSISTENT WITH SPECIAL RELATIVITY ⇒ INFINITELY LOCALIZED INITIAL STATE DOES NOT MAKE PHYSICAL SENSE.

⇒ ANY NON-RELATIVISTIC THEORY IS AN APPROXIMATION, BREAKS DOWN FOR SPEEDS $V \simeq C$

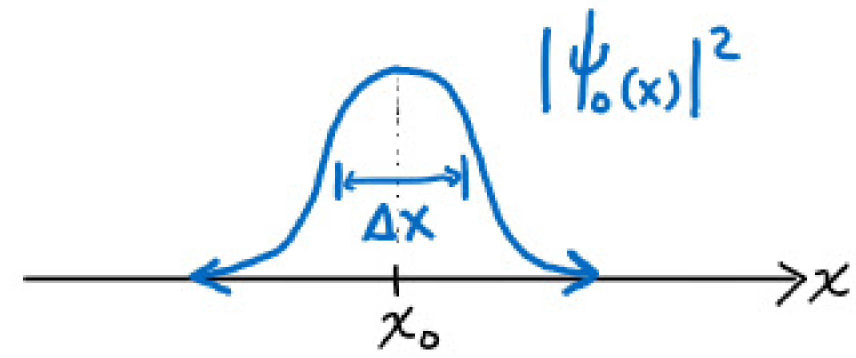
## ② THE PROPAGATOR AS A RESPONSE (GREEN'S) FUNCTION

$$\langle x|\psi(t)\rangle = \langle x|\hat{U}(t)|\psi_0\rangle = \int_{-\infty}^{\infty} dx' \, \langle x|\hat{U}(t)|x'\rangle\langle x'|\psi_0\rangle = \int_{-\infty}^{\infty} dx' \, U(x,x';t)\, \psi_0(x')$$

∴ IF WE KNOW INITIAL STATE $\psi_0(x)$, CAN GET $\psi(x,t)$ VIA CONVOLUTION ("MATRIX MULTIPLICATION") USING $U(x,x';t)$!

## Gaussian Wavepacket

$$\psi_0(x) = \frac{1}{(\pi\Delta_0^2)^{1/4}}\, e^{\frac{i P_0(x-x_0)}{\hbar}}\, e^{-\frac{(x-x_0)^2}{2\Delta_0^2}} \quad ; \quad |\psi_0(x)|^2 = \frac{1}{(\pi\Delta_0^2)^{1/2}}\, e^{-\frac{(x-x_0)^2}{\Delta_0^2}}$$




$$\int_{-\infty}^{\infty} dx\, |\psi_0(x)|^2 = 1, \quad \text{PROPERLY NORMALIZED.}$$

LEC. 9, p. 2 :

① $\langle \hat{X} \rangle = x_0$     ③ $\langle \hat{P} \rangle = P_0$

② $\Delta X = \frac{\Delta_0}{\sqrt{2}}$     ④ $\Delta P = \frac{\hbar}{\Delta_0\sqrt{2}}$

$\Rightarrow \Delta X \, \Delta P = \frac{\hbar}{2}$

SATURATES UNCERTAINTY BOUND
("MINIMUM UNCERTAINTY" WAVE PACKET)

## INITIAL PROBABILITY CURRENT:

$$J = \frac{\hbar}{m}\, \mathrm{Im}\left[\psi^* \frac{d}{dx}\psi\right] = |\psi_0(x)|^2 \times \left[\frac{P_0}{m}\right] = \begin{pmatrix}\text{PROB.}\\ \text{DENSITY}\end{pmatrix} \times \begin{pmatrix}\text{AVG.}\\ \text{VELOCITY}\end{pmatrix} \checkmark$$

## TIME EVOLUTION:

$$\psi(x,t) = \int_{-\infty}^{\infty} dx' \, U(x,x';t)\, \psi_0(x')$$

$$= \int_{-\infty}^{\infty} dx' \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} e^{\frac{im(x-x')^2}{2\hbar t}}\, \frac{1}{(\pi\Delta_0^2)^{1/4}}\, e^{i\frac{P_0}{\hbar}(x'-x_0)}\, e^{-\frac{(x'-x_0)^2}{2\Delta_0^2}}$$

ANOTHER (TEDIOUS) GAUSSIAN INTEGRAL ; RESULT :

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$$\psi(x,t) = \frac{1}{\pi^{1/4}} \left(\frac{1}{\Delta_0[1+i\lambda(t)]}\right)^{1/2} e^{-\frac{\left(x-x_0-\frac{P_0 t}{m}\right)^2}{2\Delta_0^2[1+i\lambda(t)]}}\, e^{\frac{iP_0}{\hbar}\left(x-x_0-\frac{P_0 t}{2m}\right)}$$

$$|\psi(x,t)|^2 = \frac{1}{\pi^{1/2}}\, \frac{1}{\Delta_0\sqrt{1+\lambda^2(t)}}\, e^{-\frac{\left(x-x_0-\frac{P_0 t}{m}\right)^2}{\Delta_0^2(1+\lambda^2(t))}} \quad ; \quad \lambda(t) \equiv \frac{\hbar t}{m\Delta_0^2}$$

① $\langle\psi(t)|\hat{X}|\psi(t)\rangle = \int_{-\infty}^{\infty} dx\, |\psi(x,t)|^2 x = x_0 + \left(\frac{P_0}{m}\right)t = \langle\hat{X}\rangle(t{=}0) + \langle\hat{P}\rangle_{(t=0)} \times \frac{t}{m}$ $\Longrightarrow$ BALLISTIC PROPAGATION WITH AVERAGE INITIAL VELOCITY

$$\left.\begin{array}{l} \bullet \text{ IN FACT, } \bullet \langle\psi(t)|\hat{P}|\psi(t)\rangle = \langle\hat{P}\rangle(t) = \langle\hat{P}\rangle_{(0)} = P_0 \\ \bullet\ \Delta P(t) = \left[\langle\psi(t)|\,\hat{P}^2 - \langle\hat{P}\rangle^2\,|\psi(t)\rangle\right]^{1/2} = \Delta P(0) = \frac{\hbar}{\Delta_0\sqrt{2}} \end{array}\right\} \underline{\text{WHY?}}$$

② $\Delta X(t) = \left[\langle\psi(t)|\,\hat{X}^2 - \langle\hat{X}\rangle^2(t)\,|\psi(t)\rangle\right]^{1/2} = \frac{\Delta_0}{\sqrt{2}}\sqrt{1+\lambda^2(t)}$ ; $\lambda(t) = \frac{\hbar t}{m\Delta_0^2}$ UNCERTAINTY IN POSITION INCREASES WITH TIME (FOR $\hbar \neq 0$!)

$$\Longrightarrow \Delta X(t)\,\Delta P(t) = \Delta X(0)\,\Delta P(0) \times \sqrt{1+\lambda^2(t)}$$
$$= \frac{\hbar}{2}\sqrt{1+\lambda^2(t)}$$

• LONG-TIME LIMIT: $\Delta X(t) \simeq \frac{\Delta_0}{\sqrt{2}}\lambda(t) + \mathcal{O}\left(\frac{1}{t}\right) = \frac{\hbar t}{m\Delta_0\sqrt{2}} = \frac{\Delta P}{m}\cdot t$

$\Longrightarrow$ AS $t \to \infty$, UNCERTAINTY IN POSITION = (INITIAL UNCERTAINTY IN $\underline{\text{VELOCITY}}$) × TIME!

$\therefore$ FINITE POSITION-SPACE WIDTH $\Delta_0 \Longrightarrow$ INITIAL DISTRIBUTION OF VELOCITIES HAS WIDTH

$$\frac{\Delta P}{m} = \frac{\hbar}{m\Delta_0\sqrt{2}}$$

FREE PARTICLE: $[\hat{H}, \hat{P}] = 0$

$$\hat{U}(t) = \int_{-\infty}^{\infty} dp\, |p\rangle\langle p|\, e^{-i\frac{p^2 t}{2m\hbar}}$$ $\Longrightarrow$ EVERY MOMENTUM COMPONENT EVOLVES INDEPENDENTLY

$\underline{\text{PLOTS}}$: $|\psi(x,t)|^2$ FOR $P_0 = 0$ (PURE SPREADING DUE TO VELOCITY UNCERTAINTY)

• FOUR DISCRETE VALUES OF THE DIMENSIONLESS TIME PARAMETER $\lambda = \frac{\hbar t}{m\Delta_0^2}$