Momentum vs. Wavevector

• Instead of momentum, it is often convenient to use wavevector states:

Wavevector definition: $K = \frac{P}{\hbar}$ Important commutators: [X, K] = i [P, K] = 0Eigenvalue equation: $K|k\rangle = k|k\rangle$ Relation to momentum eigenstates: $|k\rangle = c|p\rangle|_{p=\hbar k}$ $\langle k|k'\rangle = \delta(k-k')$ Normalization $\int_{-\infty}^{+\infty} dk |k\rangle \langle k| = 1$ Closure $\langle x|k\rangle = \frac{e^{ikx}}{\sqrt{2\pi}}$ Wavefunction

$$\left\langle p \left| p' \right\rangle = \delta(p - p') = \delta(\hbar k - \hbar k') = \frac{1}{\hbar} \delta(k - k') = \frac{1}{\hbar} \left\langle k \left| k' \right\rangle \right. \\ \left. \left. \left. \left| k \right\rangle = \sqrt{\hbar} \right| p \right\rangle \right|_{p = \hbar k}$$

Wavefunction in K-space

• What is the wavefunction in K-basis?

Let
$$|\psi(0)\rangle = |k_0\rangle$$

Then: $|\psi(t)\rangle = e^{-i\frac{\hbar k_0^2}{2M}t}|k_0\rangle$

$$\psi(k,t) = \left\langle k \left| \psi(t) \right\rangle = e^{-i\frac{\hbar k_0^2 t}{2m}} \left\langle k \left| k_0 \right\rangle \right.$$
$$= e^{-i\frac{\hbar k_0^2 t}{2m}} \delta(k - k_0)$$



Wavefunction in X-space

 Quantum mechanical kinetic-energy eigenstate:

$$\left|\psi\left(t\right)\right\rangle = e^{-i\frac{p_{0}}{2M\hbar}t} \left|p_{0}\right\rangle$$

- Only Global phase is changing in time
- Global phase can't be observed
- Is anything actually moving?

$$\psi(x,t) = \frac{e^{i\frac{p}{\hbar}\left(x - \frac{p_0}{2M}t\right)}}{\sqrt{2\pi\hbar}} \qquad \left|\psi(x,t)\right|^2 = \frac{1}{2\pi\hbar}$$

- The spatial phase-pattern is moving, but at:

$$v = p_0/2M$$

- This is called the `phase velocity'
 - Not related to particle velocity in classical limit
- Classical free-particle motion:

$$x(t) = x_0 + vt$$
$$p(t) = p_0$$

 How can we have a `classical limit' of QM if nothing moves at v=p /M?

<u>`Motion' in QM</u>

- The answer is that in QM motion is in interference effect
- Consider a quantum-superposition of two plane-waves:

$$\begin{split} |\psi(t)\rangle &= \frac{1}{\sqrt{2}} \left[e^{-i\frac{\hbar k_0^2}{2M}t} |k_0\rangle + e^{-i\frac{2\hbar k_0^2}{M}t} |2k_0\rangle \right] \\ \psi(x,t) &= \frac{e^{ik_0\left(x - \frac{\hbar k_0}{2M}t\right)}}{2\sqrt{\pi}} + \frac{e^{i2k_0\left(x - \frac{\hbar k_0}{M}t\right)}}{2\sqrt{\pi}} \end{split}$$

$$\begin{split} \left|\psi(x,t)\right|^{2} &= \frac{1}{2\pi} \left[1 + \frac{e^{i\left(k_{0}x - \frac{3\hbar k_{0}}{2M}t\right)}}{2} + \frac{e^{-i\left(k_{0}x - \frac{3\hbar k_{0}}{2M}t\right)}}{2} \right] \\ &= \frac{1}{2\pi} \left[1 + \cos\left(k_{0}x - \frac{3\hbar k_{0}}{2M}t\right) \right] \end{split}$$

 $= \frac{1}{\pi} \cos^{2} \left[\frac{1}{2} \left(k_{0} x - \frac{3}{2} \frac{\hbar k_{0}}{M} t \right) \right]$ This is a moving `standing wave'

• The interference pattern can move!

Wavepacket formation

- Measurement of position must produce a `localized' state
 - How does this `wavepacket' then move?

Physical versus non-physical states:

- States like $|x_0\rangle$ and $|k_0\rangle$ have $\langle \psi | \psi \rangle = \infty$
- All physical states must have $\langle \psi | \psi \rangle = 1$
- CONCLUSION 1: states such as $|x_0\rangle$ and $|k_0\rangle$ are non-physical, and can therefore only be used as intermediate states in calculations
- CONCLUSION 2: Since a measurement of X produces the nonphysical state $|x_0\rangle$, such a measurement must be impossible $x = x_0 \pm \sigma$
- However, real detectors have finite resolution
 - call the resolution σ
 - Result of measurement is therefore:
 - After measurement, state vector is projected onto this subspace, as $x_{\alpha+\alpha}$

$$\left|\psi'\right\rangle = \int_{x_0-\sigma}^{x_0+\sigma} dx \left|x\right\rangle \left\langle x\left|\psi\right\rangle\right\rangle$$

– This state will be a `wavepacket' with width σ

Gaussian Wavepackets

• A proto-typical wave packet is the Gaussian state $|x_0, \sigma\rangle$, defined via:

$$\langle x | x_0, \sigma \rangle = \frac{1}{\left[\pi \sigma^2 \right]^{1/4}} e^{-\frac{(x-x_0)^2}{2\sigma^2}}$$

- Has width σ , centered at $x=x_0$
- The width σ can be arbitrarily small, but we will always have $\langle\psi|\psi\rangle{=}1$
- Such wavepackets are the physical `position' states
- A wavepacket centered at x₀ and moving with velocity v=p₀/m, has the wavefunction:

$$\langle x | x_0, p_0, \sigma \rangle = \frac{1}{\left[\pi \sigma^2\right]^{1/4}} e^{-\frac{(x-x_0)^2}{2\sigma^2} + i\frac{p_0x}{\hbar}}$$

• How does the initial state $|x_0, p_0, \sigma\rangle$ evolve in time?

Analytic solution exists: $\psi(x,t) = \left[\pi \left(\sigma + \frac{i\hbar t}{m\sigma}\right)^2\right]^{-1/4} e^{-\frac{\left(x - \frac{p_0 t}{m} - x_0\right)^2}{2\sigma^2 \left(1 + \frac{i\hbar t}{m\sigma^2}\right)} + i\frac{p_0 \left(x - \frac{p_0 t}{2m}\right)}{\hbar}}{\psi(x,0)}$ $\psi(x,0) = \left\langle x \, \middle| \, x_0, \, p_0, \sigma \right\rangle$

Phase and Group Velocities

$$\psi(x,t) = \left[\pi \left(\sigma + \frac{i\hbar t}{m\sigma}\right)^2\right]^{-1/4} e^{-\frac{\left(x - \frac{p_0 t}{m} - x_0\right)^2}{2\sigma^2 \left(1 + \frac{i\hbar t}{m\sigma^2}\right)} + i\frac{p_0 \left(x - \frac{p_0 t}{2m}\right)}{\hbar}}{\pi}$$

• We can see that the phase velocity is

$$v_p = \frac{p_0}{2m}$$

• What does the *probability density* look like?

$$\left|\psi(x,t)\right|^{2} = \frac{1}{\sqrt{\pi}\sigma(t)} e^{-\frac{\left(x-x_{0}(t)\right)^{2}}{\sigma^{2}(t)}}$$

$$x_0(t) = x_0 + \frac{p_0}{m}t \qquad \sigma(t) = \sigma \sqrt{1 + \left(\frac{\hbar t}{m\sigma^2}\right)^2}$$

• We see that the center of the wavepacket moves at the velocity $v_g = \frac{p_0}{m}$

- We call this the `group velocity'

• We can see that the group velocity correlates with the velocity of a classical particle having the same momentum

Wavepacket Spreading

• The width of the Gaussian wavepacket is:

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

• Thus the timescale for wavepacket spreading is:

$$t_s = \frac{m\sigma^2}{\hbar} \qquad \sigma(t) = \sigma\sqrt{1 + (t/t_s)^2}$$

- For $t \ll t_s$ we can ignore spreading $\sigma(t) \approx \sigma$
- For t>>t_s the size of the wavepacket grows linearly in time:

$$\sigma(t) \approx \frac{\hbar}{m\sigma} t$$

- Thus `spreading' at the velocity: $\frac{v_s}{m\sigma} = \frac{\hbar}{m\sigma}$
- The smaller the wavepacket, the faster it will spread!



Electron Wavepacket

- Lets consider an electron:
 - $m = 10^{-30} \text{ kg}$
 - If position was measured using light, then the electron will at most be localized to the size of the wavelength
 - Visible light $\lambda = 10^{-7} \, \mathrm{m}$

$$t_{s} = \frac{m\sigma^{2}}{\hbar} = \frac{10^{-30} kg \cdot 10^{-14} m^{2}}{10^{-34} kg m^{2} s^{-1}} = 10^{-10} s$$

 Electron wavepacket will start spreading 0.1 ns after being localized

$$v_s = \frac{\hbar}{m\sigma} = \frac{10^{-34} \, kg \, m^2 \, s^{-1}}{10^{-30} \, kg \cdot 10^{-7} \, m} = 10^3 \, \frac{m}{s} = 1 \frac{km}{s}$$

- Spreading velocity, 1 km/s, is fairly large
- Hard to keep an electron pinned down to a deterministic position
 - → Classical Mechanics will not describe physics correctly
 - Repeated measurement of the electrons position could maintain localization, but random nature of measurements would introduce `quantum Brownian motion' so that CM will still not be correct

Wavepacket for a Baseball

- Here we have m = 1 kg
 - Let us still consider the center-of-mass of the electron to be localized by neutron diffraction to .1 nanometer

$$t_s = \frac{m\sigma^2}{\hbar} = \frac{1kg \cdot 10^{-20}m^2}{10^{-34}kg m^2 s^{-1}} = 10^{14}s$$

• So the wavepacket will only start spreading after 10^{14} s = 30 million years

$$v_s = \frac{\hbar}{m\sigma} = \frac{10^{-34} \, kg \, m^2 \, s^{-1}}{1 kg \cdot 10^{-10} \, m} = 10^{-24} \, \frac{m}{s} \qquad \frac{1 \, \text{nm}}{300 \, \text{million years}}$$

 After which it will start to spread at a rate of 10⁻²⁴ m/s.

In another 30 million years, it will have doubled in size

- Note: the age of the universe is 13 billion years
- In that time it will have reached 10 nm.
- So classical mechanics (i.e. welldefined/deterministic position and momentum) should do pretty well