# Quantum Physics 1

Notes-4

The wavefunction and its interpretation

Probability current

The wave packet

Space and momentum representations

Heisenberg Uncertainty Principle

# Important results so far

Einstein− deBroglie relations: $p = \hbar k = \frac{h}{\lambda}$; $\quad E = \hbar\omega = hf$

The probability interpretation: $\quad P(x)dx = \Psi^*\Psi dx$

$$\langle q \rangle = \int \Psi^* q(x) \Psi dx$$

The standard deviation of a distribution is:

$$\sigma = \sqrt{< x^2 > - < x >^2}$$

The general form for a wave packet using waves with

well−defined momentum: $\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{\infty} A(k) e^{i(kx-\omega t)} dk$

where $A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} dx$ and $P(k)dk = A^* A dk$

# Class 4 In-Class Activity

a) Assume that the wavefunction of a square pulse at time zero is

$$\Psi(x,0) = \begin{cases} 0 \; for \; x < -a \\ \dfrac{1}{\sqrt{2a}} \;\; for \; -a < x < a \\ 0 \; for \; x > a \end{cases}$$

b) Find the standard deviation $\sqrt{\langle x^2 \rangle - \langle x \rangle^2}$ of this distribution.

c) Find $A(k)$

d) Find the standard deviation of $A(k)$.

e) Does this wavefunction obey the Heisenberg Uncertainty Principle?

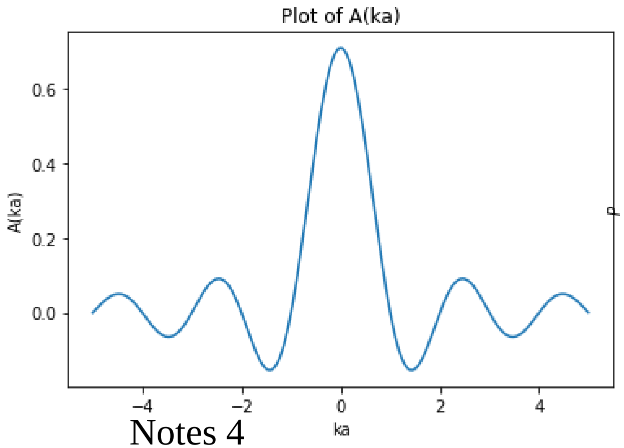
# Comments: Class 4 Activity

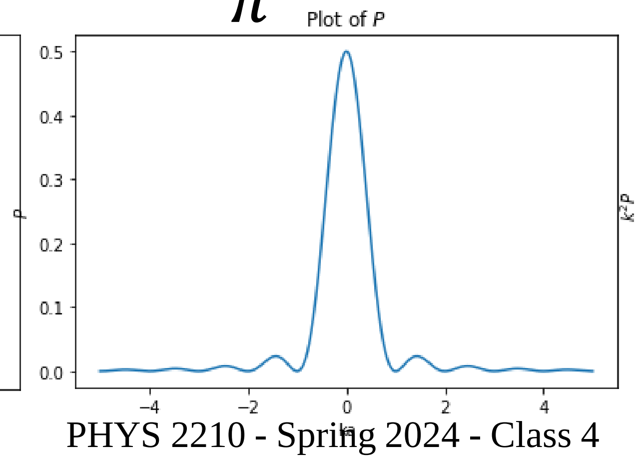
$$A(k) = \frac{1}{\pi\sqrt{4a}}\int_{-a}^{a} e^{ikx}dx = \frac{i}{\pi\sqrt{4a}}\frac{\left(e^{-ika} - e^{ika}\right)}{k}$$

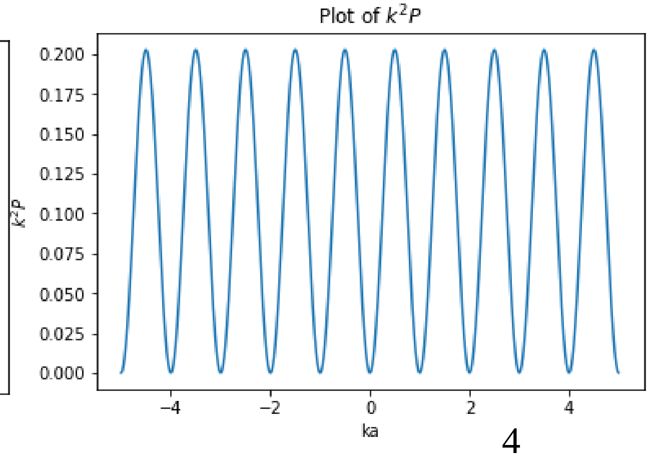
$$= \frac{2a}{\pi\sqrt{4a}}\frac{\left(e^{ika} - e^{-ika}\right)}{2iak} = \frac{\sqrt{a}}{\pi}\frac{\sin(ka)}{ka}$$

So the probability density for finding the state with a momentum wavevector k is:

$$A^*A = \frac{a}{\pi^2}\, sinc^2(ka)$$



# Conservation of Probability

It is important that the total probability of finding a particle does not change with time.

Is this consistent with the Schrodinger equation?

- First calculate the time derivative of the probability density:

$$\frac{\partial P}{\partial t} = \frac{\partial \Psi^* \Psi}{\partial t} = \Psi^* \frac{\partial \Psi}{\partial t} + \Psi \frac{\partial \Psi^*}{\partial t} \quad (1)$$

- And from the SE:

$$\frac{\partial \Psi}{\partial t} = \frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi\right) \text{ and } \frac{\partial \Psi^*}{\partial t} = \frac{-1}{i\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi^*}{\partial x^2} + V(x)\Psi^*\right)$$

and substituting space derivatives for time derivatives in (1):

$$\frac{\partial P}{\partial t} = \Psi^* \frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi\right) - \Psi \frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi^*}{\partial x^2} + V(x)\Psi^*\right)$$

$$\frac{\partial P}{\partial t} = \frac{\mathrm{i}\hbar}{2m}\left(\Psi^* \frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} - \Psi \frac{\hbar^2}{2m}\frac{\partial^2 \Psi^*}{\partial x^2}\right) = \frac{\mathrm{i}\hbar}{2m}\frac{\partial}{\partial x}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x}\right)$$

# Conservation of probability

From the previous page: $\frac{\partial P}{\partial t} = \frac{\mathrm{i}\hbar}{2m}\frac{\partial}{\partial x}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x}\right)$

So  the rate of change of the total probability is:

$$\frac{\partial}{\partial t}\int P dx = \int \frac{\partial P}{\partial t} dx = \frac{i\hbar}{2m}\int_{-\infty}^{\infty} \frac{\partial}{\partial x}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x}\right) dx$$

$$\frac{\partial}{\partial t}\int P dx = \frac{i\hbar}{2m}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x}\right)\Bigg|_{-\infty}^{\infty} = 0$$

The final step is because in order to be normalizable the wavefunction must go to zero at $\pm\infty$.

THUS, IF THE WAVEFUNCTION IS A SOLUTION TO THE SE AND IS NORMALIZABLE, THEN PROBABILITY IS CONSERVED.

# Probability Current

- The probability current density
$$-\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x}-\Psi\frac{\partial\Psi^*}{\partial x}\right)\equiv j_x(x)$$
is a useful concept that helps in thinking about traveling particles.

# Probability Current for a Pure Momentum Function

$$\Psi_{p0}(x,t) = Ae^{i(p_0 x - Et)/\hbar}$$

$$j_x(x) = -\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right)$$

$$= -\frac{i\hbar}{2m}\left(\frac{A^*Aip_0}{\hbar} - \left(-\frac{A^*Aip_0}{\hbar}\right)\right)$$

$$= \frac{|A|^2 p_0}{m} = |A|^2 v_0$$

(Makes sense.)

Note that $\frac{\partial}{\partial t}P([a,b],t) = j_x(a) - j_x(b) = 0$ for this case.

# In class activity (not to be handed in)

- Evaluate the probability current for the wave function $\Psi = Ae^{ikx+\omega t} + Be^{-ikx+\omega t}$

- Each group should develop an answer and be prepared to present it to me.

# Particles and waves: the Gaussian wavepacket

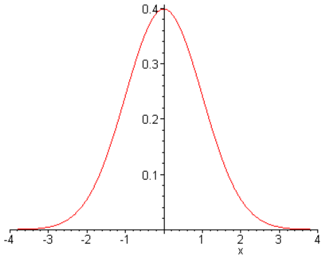
We will simplify calculations by assuming that the spatial part of the wavefunction can be described at $t = 0$ by a Normal Gaussian function centered at $x_0$ and moving with average wavenumber $k_0$;

$$\Psi(x,0) = \left(\frac{1}{\sigma_x\sqrt{2\pi}}\right)^{1/2} e^{ik_0x} e^{-(x-x_0)^2/4\sigma_x^2}.$$

(We have already solved a similar problem in Notes 2. )

So $A(k) = \frac{1}{\sqrt{2\pi}}\left(\frac{1}{\sigma_x\sqrt{2\pi}}\right)^{1/2} \int\limits_{-\infty}^{\infty} e^{i(k_0-k)x} e^{-(x-x_0)^2/4\sigma_x^2} dx$

# Gaussian wavepacket continued




to simplify further let's take $x_0 = 0$,

$$\text{so } A(k) = \frac{1}{\sqrt{2\pi}}\left(\frac{1}{\sigma_x\sqrt{\pi}}\right)^{1/2} \int_{-\infty}^{\infty} e^{i(k_0-k)x} e^{-x^2/2\sigma_x^2} dx$$

Then letting $k' = k - k_0$, we solve by completing the square:

$$-ik'x - \frac{1}{2\sigma_x^2}x^2 + \sigma_x^2 k'^2 - \sigma_x^2 k'^2 = \left(\frac{1}{\sqrt{2}\sigma_x}x - i\sigma_x k'\right)^2 + \sigma_x^2 k'^2$$

$$A(k) = \frac{1}{\sqrt{2\pi}}\left(\frac{1}{\sigma_x\sqrt{\pi}}\right)^{1/2} e^{-\sigma_x^2 k'^2} \int_{-\infty}^{\infty} e^{-\left(\frac{1}{2\sigma_x}x - i\sigma_x k'\right)^2} dx$$

$$\text{let } x' = \frac{x}{\sqrt{2}\sigma_x} - i\sigma_x k', \text{ then } A(k) = \frac{1}{\sqrt{2\pi}}\left(\frac{1}{\sigma_x\sqrt{\pi}}\right)^{1/2} \sqrt{2}\sigma_x e^{-\sigma_x^2 k'^2} \int_{-\infty}^{\infty} e^{-x'^2} dx'$$

$$A(k) = \frac{1}{\sqrt{2\pi}}\left(\frac{1}{\sigma_x\sqrt{\pi}}\right)^{1/2} \sqrt{2}\sigma_x e^{-\sigma_x^2 k'^2}\sqrt{\pi} = \left(\frac{1}{\pi}\sigma_x^2\right)^{\frac{1}{4}} e^{-\frac{\sigma_x^2(k-k_0)^2}{2}}$$

# Gaussian wavepacket continued

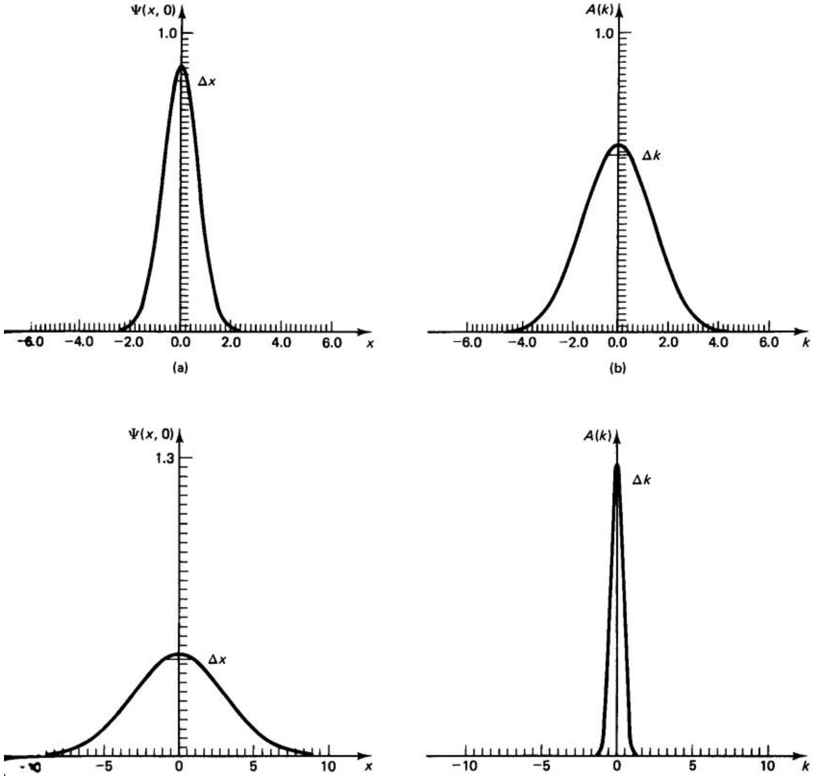
$$A(k) = \left(\frac{1}{\pi}\sigma_x^2\right)^{\frac{1}{4}} e^{-\frac{\sigma_x^2(k-k_0)^2}{2}}$$

This is a Normal Gaussian $k-$distribution,

centered at $k_0$ with width $\sigma_k = \frac{1}{\sigma_x}$.

- Although we specified a wave momentum $k_0$ we find that the wavefunction actually contains a spread of wave momenta, $\frac{1}{\sigma_x}$, which increases as the spatial Gaussian narrows. Remember that $\Delta k = \frac{\Delta p}{\hbar}$.
- Waves of differing k move at different speeds, so the original wavefunction will spread with time.

# Inversely correlated widths




Note that if $\Psi$ is properly normalized ($\int \Psi^* \, \Psi dx = 1$)

then the wavevector amplitude function is also normalized to 1:

$$\int |A(k)|^2 dk = 1$$

# An aside on the definition of the width of a Gaussian

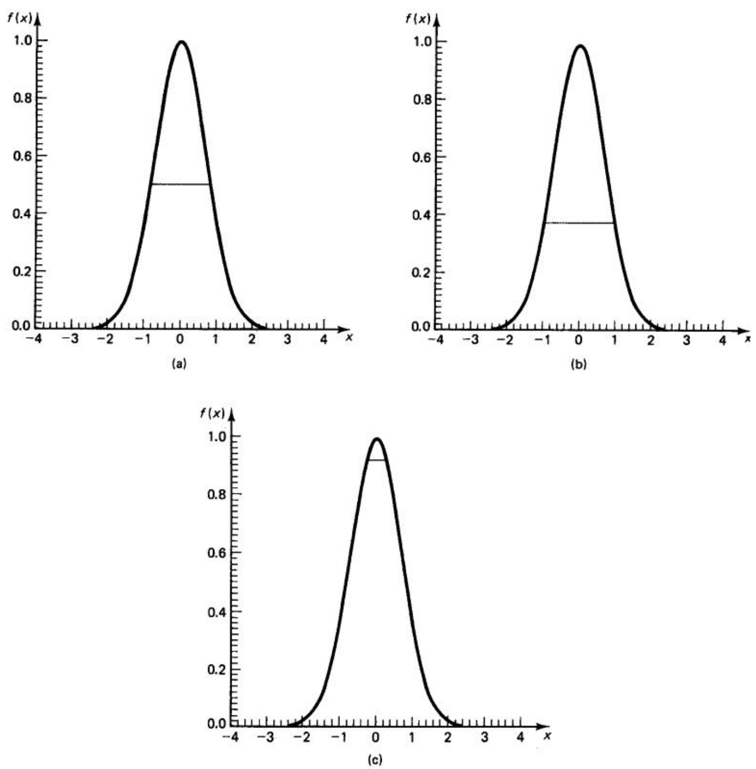



**Figure 4.8** A cornucopia of definitions of the width $w_x$ of a function $f(x)$. The function at hand is $f(x) = e^{-x^2}$. (a) The full-width-at-half-maximum, $w_x = 1.665$. (b) The extent of the function at the special point where $f(x) = [f(x)]_{\max}/e$. The function $e^{-x^2}$ is equal to $1/e$ of its maximum value at $x = \pm 1$, so this definition gives $w_x = 1.736$. (c) My definition: the standard deviation of $x$; for this function, $w_x = \Delta x = 0.560$.

The width of a Gaussian can be defined in various ways. Two conventional ways are by the Full Width at Half Maximum (FWHM) and twice the standard deviation. Morrison uses ΔL=standard deviation of the position.

# Time evolution of the wavefunction

The general form of the wavefunction is:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{-i(kx-\omega t)} dk.$$

This means that if you are given $\Psi(x,0)$ you can find $\Psi(x,t)$.

$$A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-i(kx)} dx.$$

To do the top integral, you must know $\omega(k)$.

The simplest case is for a pulse of light, $\omega = kc$

$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{-ik(x-ct)} dk.$

which produces a travelling pulse that does not change shape as a function of time.

# Group velocity for a wave-packet

$$\psi(x,t) = \int A(k) e^{-i(kx-\omega(k)t)} dk$$

Assuming that $A(k)$ has a fairly narrow range of important $k'$s.
we will allow ourselves to expand $\omega(k)$:

$$\omega(k) \cong \omega(k_0) + (k-k_0)\left(\frac{d\omega}{dk}\right)_{k_0} + \ldots$$

Letting $k' = k - k_0$

$$\psi(x,t) \cong e^{i(k_0 x - \omega(k_0)t} \int dk'\, e^{-ik'\left[x - \left\{\frac{d\omega}{dk}\right\}t\right]_0}$$

Therefore in this simple expansion, the group velocity is just

$$v_g = \frac{d\omega}{dk}$$

# Momentum Probability Amplitude

Note that $A(k)$ clearly contains information about momentum because $k = p/\hbar$.

It is useful (later) to be able to describe the state function directly in terms of momentum states.

$\Phi(p) \equiv \frac{1}{\sqrt{\hbar}} A\left(\frac{p}{\hbar}\right)$ (the momentum probability amplitude)

Then we can rewrite the wavefunction as;

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Phi(p) e^{ipx/\hbar} dp \quad \text{and}$$

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ipx/\hbar} dx.$$

Note that the factor of $1/\sqrt{\hbar}$ is required for proper normailzation of $\Psi$ and $\Phi$.

# Interpretation of the space and momentum state functions

$\Psi(x,t)$ = the wavefunction and directly gives information about the probability of finding a particle at a specific position, but it is difficult to directly calculate properties like the expected momentum because momentum is not written as a function of position.

$\Phi(p)$ = the momentum probability amplitude and directly gives information about the probability of finding a particle with a specific momentum.

They both describe the same quantum state.

If the members of an ensemble are in the quantum state $\Psi$(x,t)
with Fourier transform $\Phi(p) = F[\Psi(x,0)]$ then
$P(p)dp = \Phi * (p)\Phi(p)dp$
is the probability that in a momentum measurement at time $t$ a particle's momentum will be found to be between $p$ and $p + dp$.

# Expectation values

Given the momentum amplitude function and the associated probability distribution, we can compute expectation values:

$$\langle p \rangle = \int_{-\infty}^{\infty} \Phi(p) * p\Phi(p)dp$$ = expectation value (average) of p.

$\Delta p =$ momentum uncertainty$=[(p - \langle p \rangle)^2]^{1/2} = [\langle p^2 \rangle - \langle p \rangle^2]^{1/2}$

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} \Phi(p) * p^2\Phi(p)dp$$

**TABLE 4.1 POSITION AND MOMENTUM INFORMATION FOR A GAUSSIAN STATE FUNCTION WITH $L = 1.0$, $x_0 = 0$, AND $p_0 = 0$**

| Position | Momentum |
|---|---|
| $\Psi(x,0) = \left(\frac{1}{2\pi L^2}\right)^{1/4} e^{-x^2/(4L^2)}$ | $\Phi(p) = \left(\frac{2}{\pi}\frac{L^2}{\hbar^2}\right)^{1/4} e^{-p^2L^2/\hbar^2}$ |
| $\langle x \rangle = 0$ | $\langle p \rangle = 0$ |
| $\Delta x = L$ | $\Delta p = \frac{1}{2L}\hbar$ |