PH 112: Quantum Physics and Applications

S. Shankaranarayanan
shanki@iitb.ac.in

Week 02 Lecture 3: Fourier transform and Uncertainty Principle

Spring 2023

Matter Waves: Recap and way-forward

de Broglie: If waves can mimic particles, then particles can mimic waves

$$\lambda = \frac{h}{m\,v} = \frac{h}{p}$$

Matter Waves

Question

If a photon has energy and momentum, why the particles can't have wave-like properties?

implies

de Broglie hypothesis → momentum of a particle $p = h/\lambda$ → implies → Wavelength of a particle $\lambda = h/p$ → Demostrated by scattering of electron in a crystal

Duality

Particles and Waves → Is Light a particle or wave? → needs → determining position and momentum → implies → Heisenberg Uncertainty principle

Fourier Transform (FT): Recap

Space

x	Spatial coordinate
L	spatial wavelength
$k = \frac{2\pi}{\lambda}$	spatial wavenumber
$F(k)$	wavenumber spectrum

Time

t	Time variable
T	period
$\omega = 2\pi s$	angular frequency
$F(\omega)$	frequency spectrum

Fourier Integrals

With the complex representation of sinusoidal functions e^{ikx} (or e^{iwt}) the Fourier transformation can be written as:

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k)\, e^{-ikx}\, dk$$

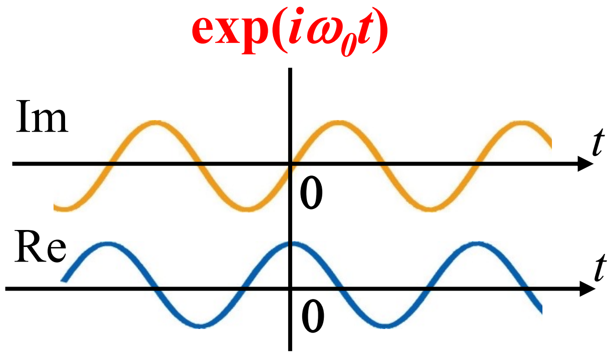
$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\, e^{ikx}\, dx$$

Another way of writing the prefactor: Distribute it to both Fourier and Inverse Fourier

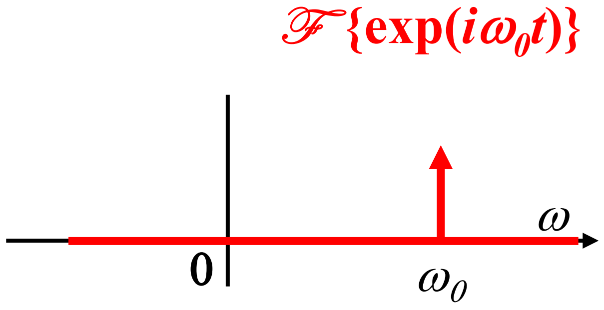
Example 1: Fourier transform of $exp(i\,\omega_0 t)$

$$F\ \{\exp(i\omega_0 t)\} = \int_{-\infty}^{\infty} \exp(i\omega_0\, t)\exp(-i\,\omega t)\, dt$$

$$= \int_{-\infty}^{\infty} \exp(-i[\omega - \omega_0]t)\, dt$$



In the frequency space, the signal has one value at $\omega = \omega_0$.



Fourier transform provides information about the signal.

Properties of Fourier Transform

	Spatial Domain *(x or t)*	Frequency Domain $u = (k, \omega)$
Linearity	$c_1 f(x) + c_2 g(x)$	$c_1 F(u) + c_2 G(u)$
Scaling	$f(ax)$	$\frac{1}{\lvert a \rvert} F\left(\frac{u}{a}\right)$
Shifting	$f(x - x_0)$	$e^{-i2\pi u x_0} F(u)$
Symmetry	$F(x)$	$f(-u)$
Conjugation	$f^*(x)$	$F^*(-u)$
Convolution	$f(x) * g(x)$	$F(u)G(u)$
Differentiation	$\frac{d^n f(x)}{dx^n}$	$(i2\pi u)^n F(u)$

Note that these are derived using frequency ($e^{-i2\pi ux}$)

Scale theorem in Fourier transform

Scale theorem in Fourier Transform

FT of a scaled function $f(a\,t)$ $(a \neq 0)$

$$\mathrm{F}\ \{f(at)\} = F(\omega/a)\ /\ |a|$$

Proof $$\mathrm{F}\ \{f(at)\} = \int_{-\infty}^{\infty} f(at)\exp(-i\omega t)\,dt$$

Assume $a > 0$, change variables: $u = at$

$$\mathrm{F}\ \{f(at)\} = \int_{-\infty}^{\infty} f(u)\exp(-i\omega[u/a])\,du\ /\ a$$

$$= \int_{-\infty}^{\infty} f(u)\exp(-i\,[\omega/a]\,u)\,du\ \ /\ \ a$$

$$= F(\omega/a)\ /\ a$$

If $a < 0$, the limits flip when we change variables, introducing a minus sign, hence the absolute value.

Three cases:

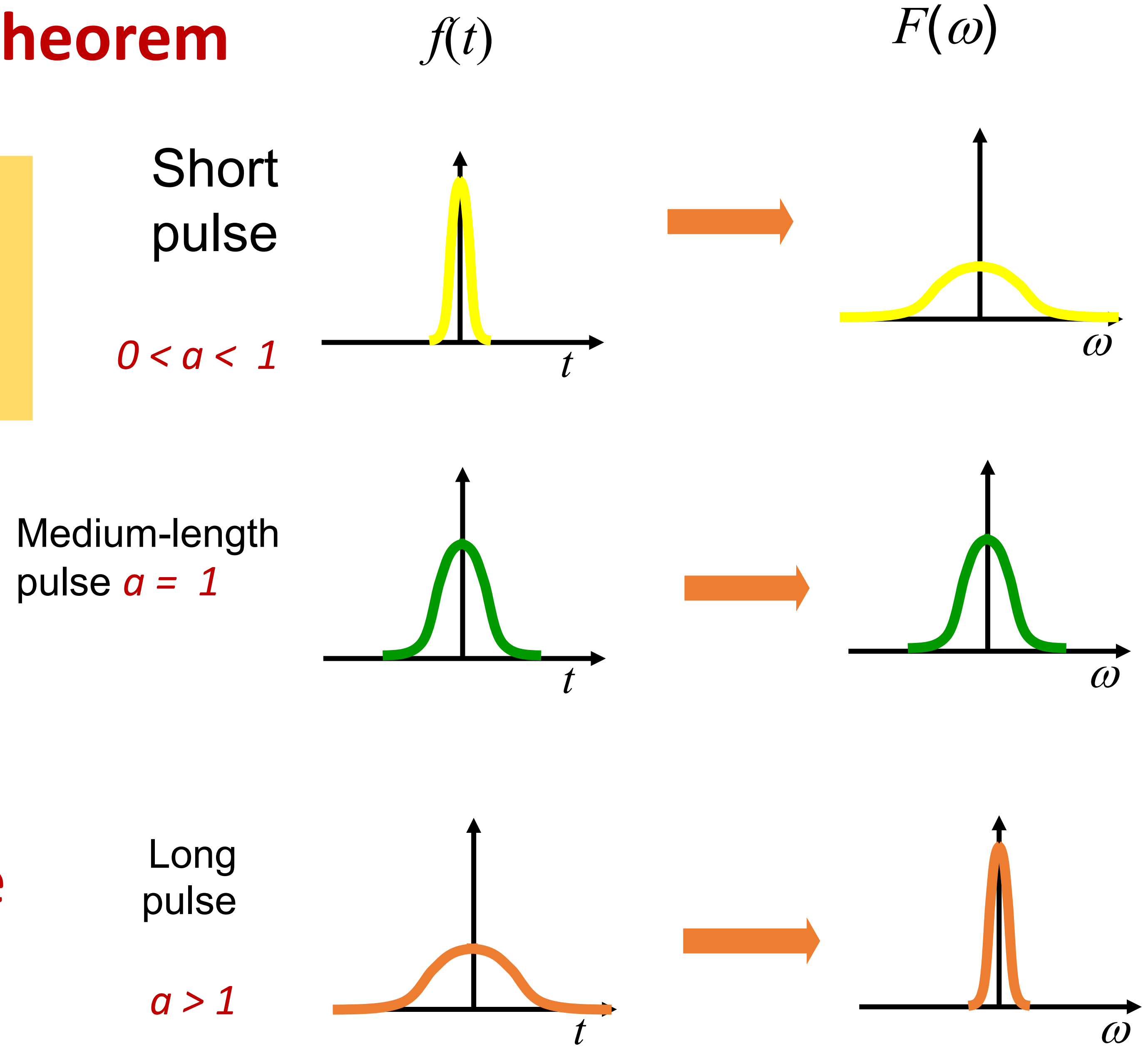
1. $0 < a < 1$
2. $a = 1$
3. $a > 1$

Consequence of Scale Theorem

Shorter the pulse ($\Delta t \downarrow$), broader the bandwidth ($\Delta\omega \uparrow$) !

Cannot simultaneously reduce time duration and bandwidth!

This is the essence of the Uncertainty Principle!



Uncertainty Principle in FT

- A signal cannot be arbitrarily narrow in time and in frequency.

FT increases in spread as the time sequence decreases in width.

- This property of FT is formalized with the Uncertainty Principle:

Formal definitions are needed of the width of a signal and it's FT. They are referred to as duration, D(x), and bandwidth, B(x), respectively:

Matter Waves

Principle of Superposition of waves: Recap

- When two or more waves traverse the same region, they act independently of each other.

- Consider two cosine waves with very similar frequency $(\omega_1 \simeq \omega_2)$ and wave number $(k_1 \simeq k_2)$. We have:

cos

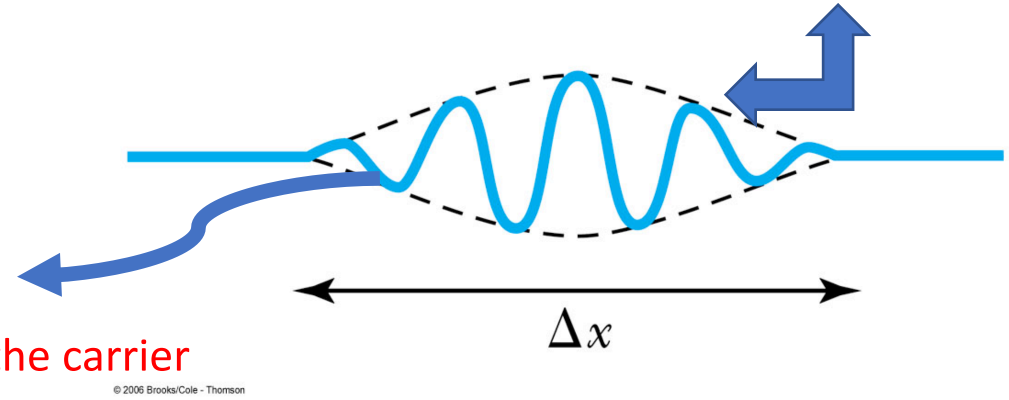
$$\Psi(x,t) = \Psi_1(x,t) + \Psi_2(x,t) = 2A\left(\frac{\Delta k}{2}x - \frac{\Delta\omega}{2}t\right)\cos(k_{\mathrm{av}}x - \omega_{\mathrm{av}}t)$$

- When many more waves are combined, the phase of the wave oscillates within an envelope that denotes the maximum displacement of the combined waves.

- When combining (infinitely many) waves with different amplitudes and frequencies and wave numbers, a pulse, or **wave packet**, is formed which moves at a **group velocity**:

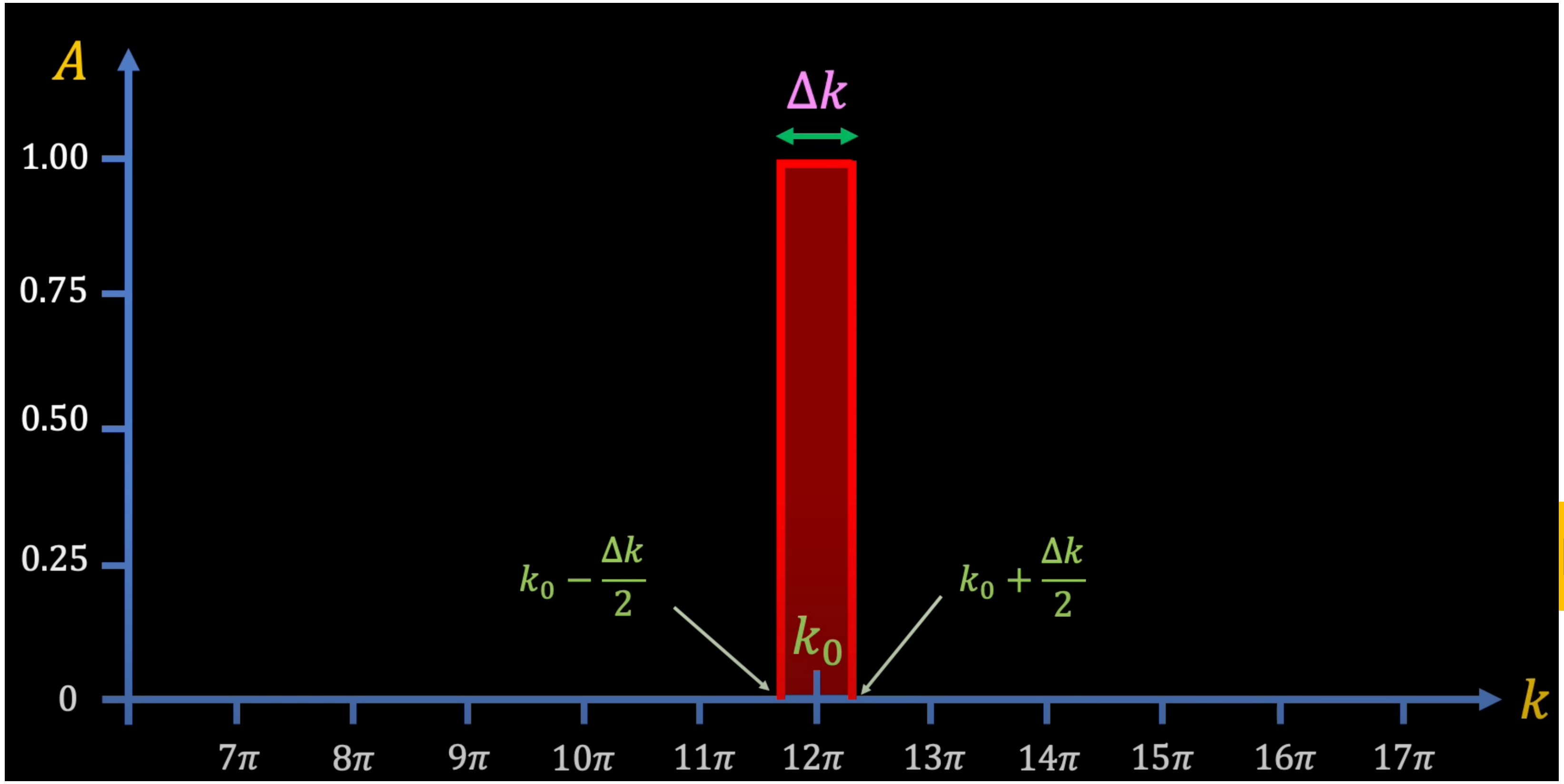
$$v_{group} = \frac{\Delta\,\omega}{\Delta\,k}$$

Speed at which the envelope moves



Speed of the carrier

Example 2: Wave packet



$$A(k) = \begin{cases} 0 & k_0 - \Delta k < 0 \\ 1 & k_0 - \Delta k < k < k_0 + \Delta k \\ 0 & 0 > k_0 + \Delta k \end{cases}$$

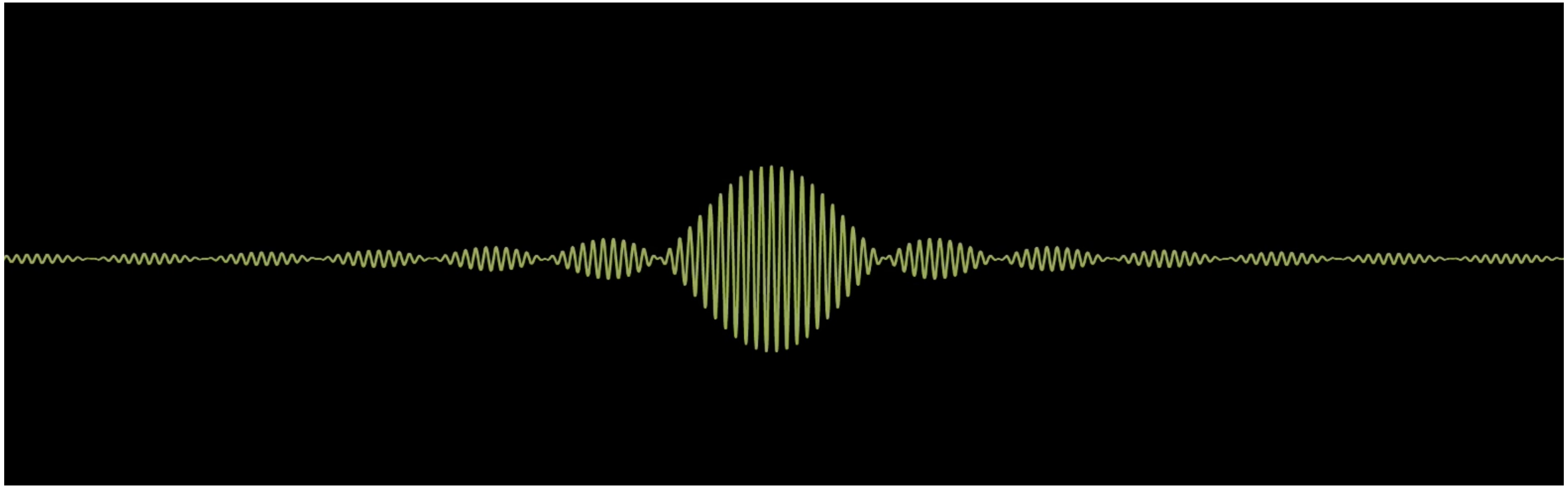
Let us not an inverse Fourier transform from the k-space to x-space.

$$F(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k)\, e^{-i k x}\, dk$$

Remember this is the same example we did in the last class, except now we are interested in obtaining the Fourier transform in x-space.

Example 2: Wave packet

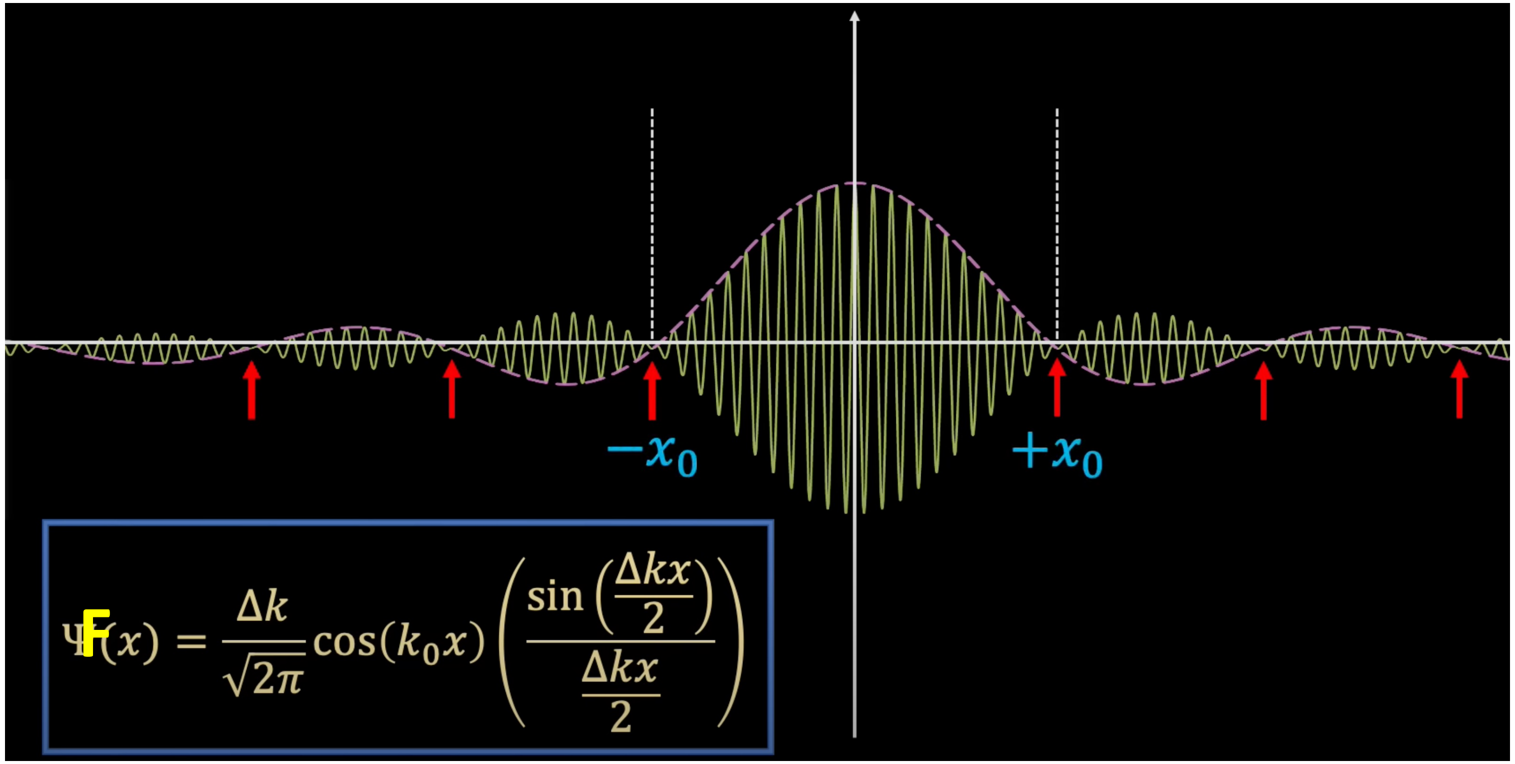
$$F(x) = \frac{\Delta k}{\sqrt{2\pi}} \cos\left(k_0 x\right) \left(\frac{\sin\left(\frac{\Delta k x}{2}\right)}{\frac{\Delta k x}{2}} \right)$$



Depending of the value of Δk, we can have a large Central lobe and small side lobes such that it corresponds to localization in space (wavepacket).

A wavepacket is a continuous distribution of waves in small region in k-space!

Wave packet



$$\sin\left(\frac{\Delta k |x_0|}{2}\right) = 0$$

central wavepacket width $\Delta x = 2\, x_0$

Question: Can we determine width?

$$\frac{\Delta k x_0}{2} = \pi \implies x_0 = \frac{2\pi}{\Delta k}$$

Δk decreases $\implies x_0$ increases

Δk increases $\implies x_0$ decreases

$$\Delta k \Delta x = 4\pi$$

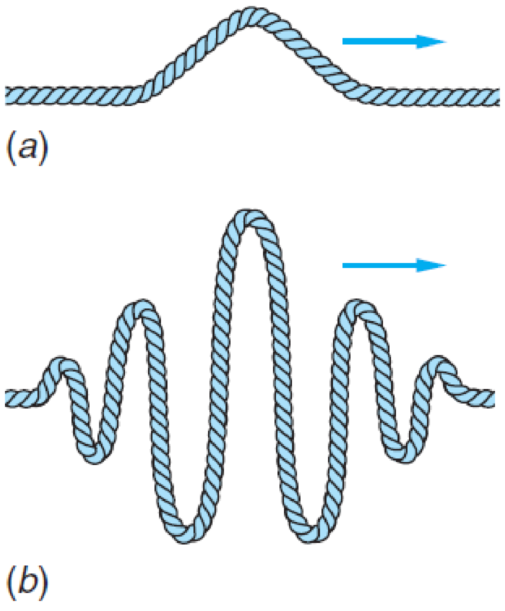
Since wave packet tells us information about where we are most likely to find our particle if the width of the wave packet increases our uncertainty in where the particle is located must also increases!

Free particle wavepacket

Free particle $$E = \frac{p^2}{2m}, p = mv$$

de Broglie relation $$E = \hbar\omega, p = \hbar k$$

This means $$\Delta p \uparrow \implies \Delta k \uparrow$$



Uncertainty in de Broglie's wavepacket $$\Delta p \Delta x = 2h$$

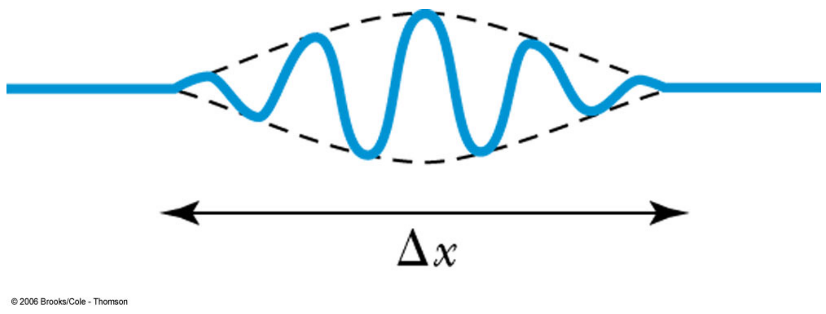
Note that this is only an estimate and not the complete expression!

$$\text{narrow packet} \implies \text{small } \Delta x;\ \text{large}\Delta p$$
$$\text{wide packet} \implies \text{large } \Delta x;\ \text{small}\Delta p$$

Heisenberg Uncertainty principle

Wave packets

An idealized wave packet



$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{ikx}\, dk$$

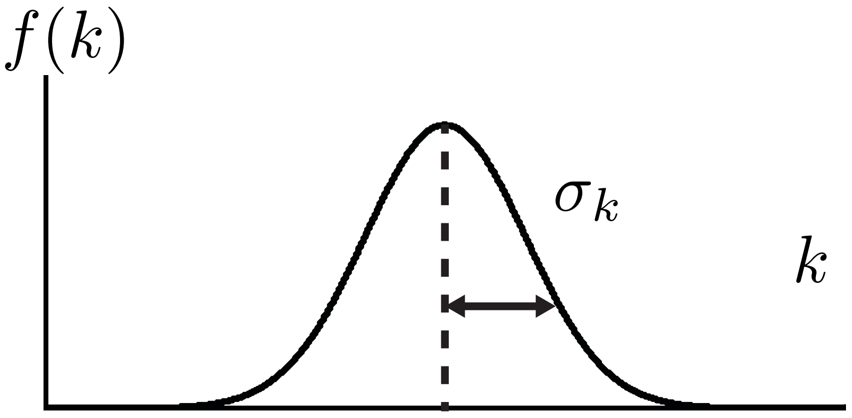
Wave packet localized in space

Broad wavenumber spectrum

Example 3: Gaussian wave packet of light

- Consider a wave packet of light moving in z-axis

$$\vec{E} = \overrightarrow{E_0} \int_{-\infty}^{\infty} f(k)\, e^{ikz}\ dk$$ (ignore t dependence)



- Assume Gaussian frequency distribution

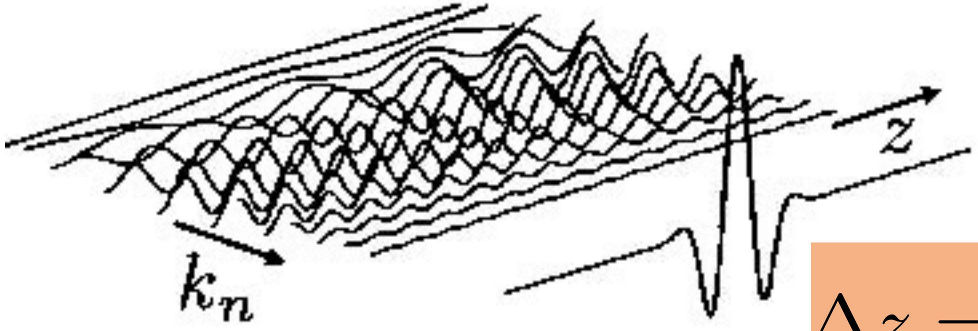
$$f(k) = \frac{1}{\sqrt{2\pi\sigma_k}} exp\left(-\frac{(k-k_o)^2}{2\sigma_k^2}\right)$$

$$\Delta k = \frac{\sigma_k}{\sqrt{2}}$$

- FT of a Gaussian is a Gaussian!

$$\boxed{\mathcal{F}_x\left[e^{-ax^2}\right](k) = \sqrt{\frac{\pi}{a}} e^{-\frac{\pi^2 k^2}{a}}}$$

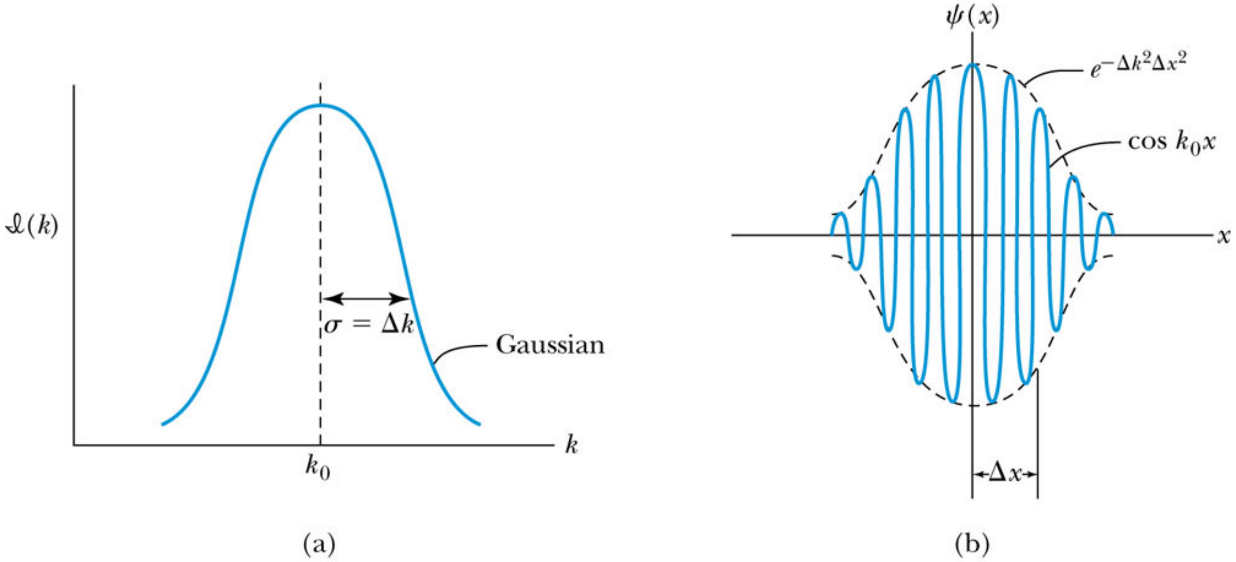
Gaussian wave packet of light and matter



$$\Delta z = \frac{1}{\sqrt{2}\sigma_k}$$

$$\boxed{\Delta k \Delta z = 1/2}$$

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(k) e^{ikx}\, dk$$



Uncertainty Principle

The Uncertainty Principle

- One of the fundamental consequences of quantum mechanics is that it is impossible to simultaneously determine the position and momentum of a particle with complete precision.

- We can understand this by thought (Gedanken) experiments

1. Measuring time using a clock

2. Single slit diffraction of a Photon

3. Heisenberg Microscope

Beats and Uncertainty principle

- Consider we have a standard clock with an oscillator that produces waves whose frequency is (ν_2).
- Consider an incoming wave with frequency (ν_1).
- We want to compare the frequency of the clock with the incoming wave frequency.
- A beat will arise if the two waves have very similar frequency $(\nu_1 \simeq \nu_2)$. Beat frequency is $\Delta\nu = \frac{\nu_1 - \nu_2}{2}$
- Time required to observe one beat is $\frac{1}{\Delta\nu}$ (period of the group frequency).
- To be confident of observing the beat, we must make measurement over time Δt which must be greater than the period of the group frequency: $\Delta t \geq \frac{1}{\Delta\nu}$
- Longer is the measurement time, smaller is the uncertainty in frequency: $\Delta t\, \Delta\nu \geq 1$

Beats and Uncertainty principle

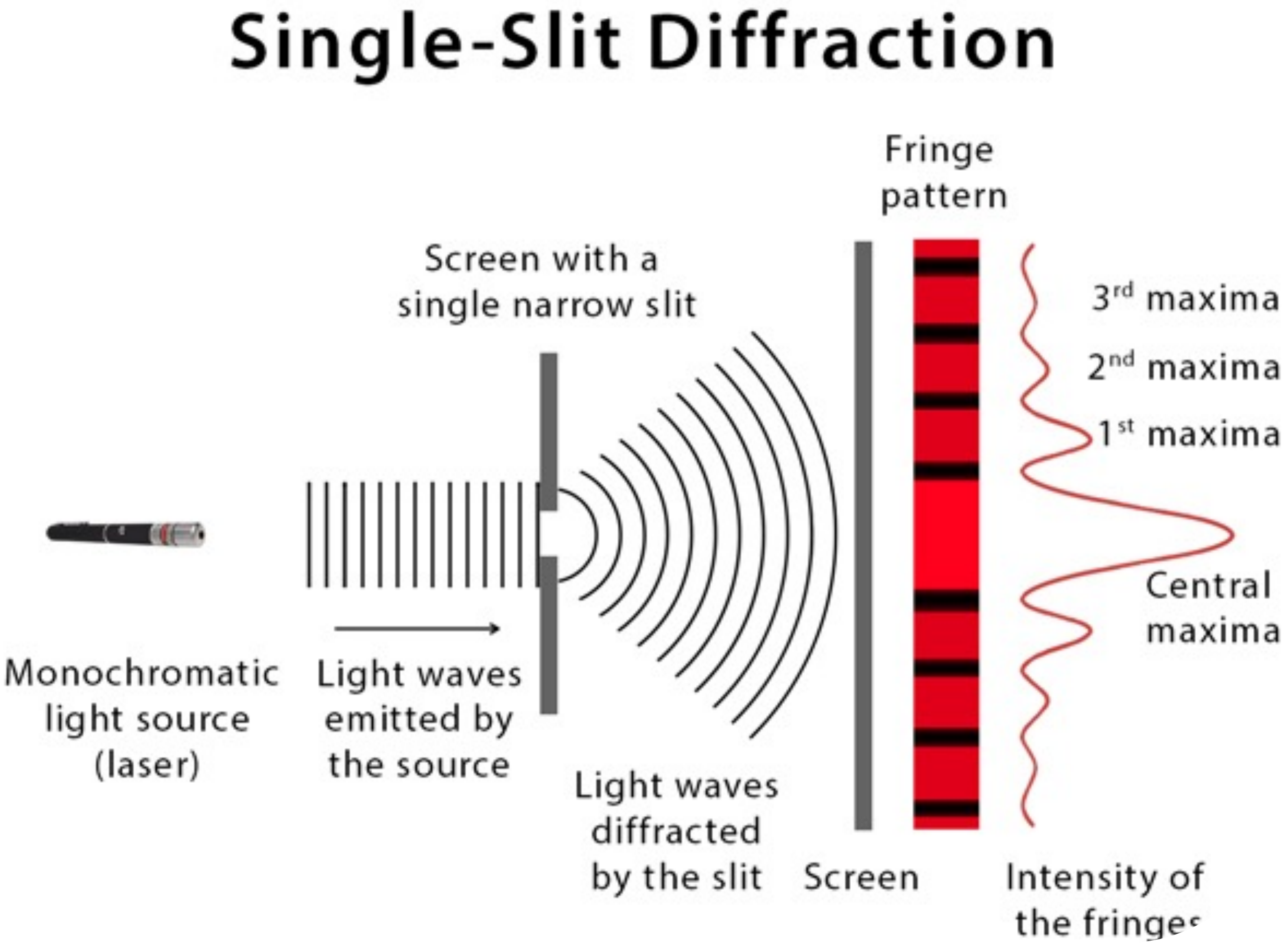
- In time Δt, the wave will move a distance Δx
- Uncertainty in the location of the wave is Δx.
- Let v be the velocity of the wave $\Longrightarrow \Delta t = \frac{\Delta x}{v}$.
- From the uncertainty relation between Δt and $\Delta \nu \;\Longrightarrow \Delta x\, \Delta \nu \geq v$
- Using the relation $v = \nu\, \lambda$, we have $\Delta \nu = \dfrac{v\, \Delta \lambda}{\lambda^2}$
- From the above two relations, we have $\Delta x\, \Delta \lambda \geq \lambda^2$
- Using the de Broglie’s relation, we have $\Delta x\, \Delta p \geq h$

Note that this is only an estimate and not the complete expression!

Single Slit Diffraction: Wave Picture

Geometrical optics picture breaks down when slit width becomes comparable to wavelength (λ).

a is width of the slit,
d is horizontal distance between the screen and slit.



Single Slit Diffraction: Wave Picture

$$\boxed{\sin\theta = \frac{m\lambda}{a}}$$

Position of dark fringes in single-slit diffraction

Let us now make small angle approximation $\sin\theta \approx \tan\theta \approx \theta = y_{min}/R$

$$\boxed{y_{\min} = \frac{Rm\lambda}{a}}$$

Positions of intensity minima (y_{min}) of diffraction pattern on screen, measured from central position.

The above expression is similar to one derived for 2-slit interference experiment:

$$y_{int} = R\,\frac{n\,\lambda}{d}$$

In the Interference experiment, y_{int} are positions of intensity maxima.

Width of central maximum

The width of the central maximum is the distance between the m = +1 minimum and the m=-1 minimum:

$$\boxed{\Delta y = \frac{R\lambda}{a} - -\frac{R\lambda}{a} = \frac{2R\lambda}{a}}$$

Narrower the slit, the more the diffraction pattern "spreads out"

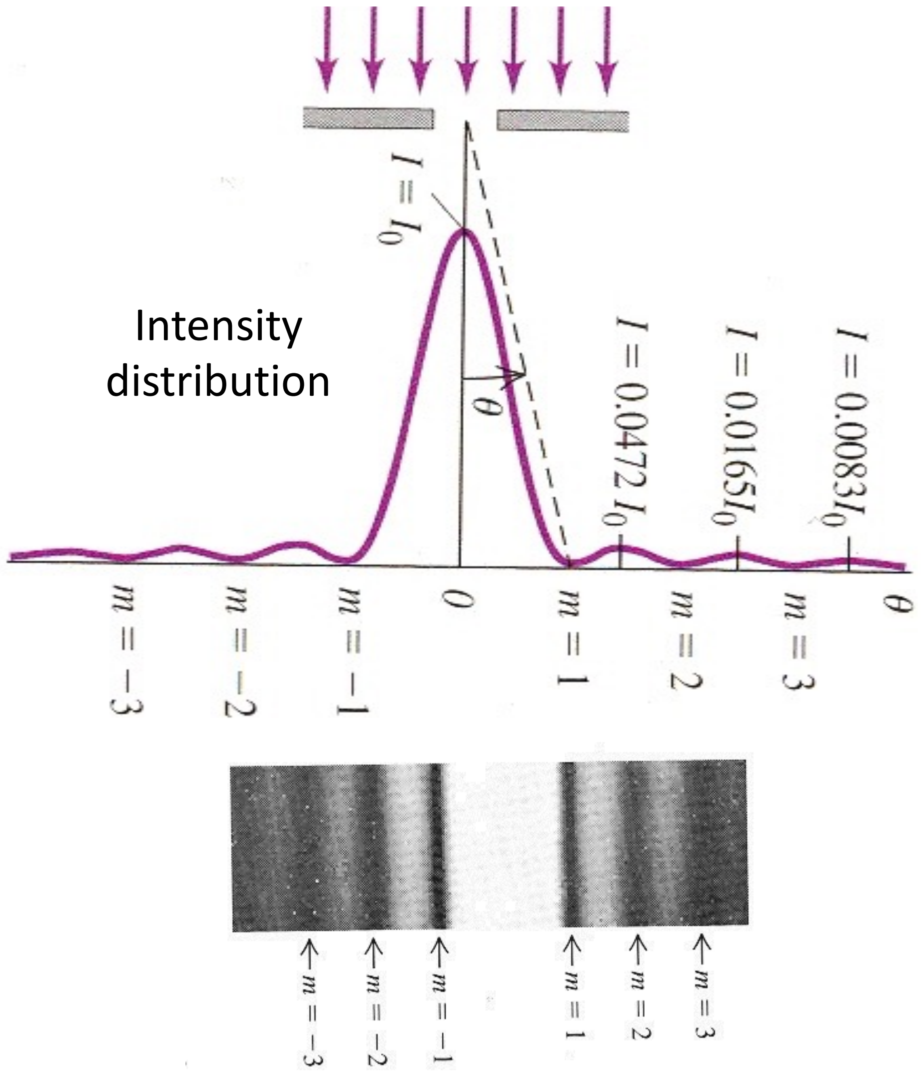


image of diffraction pattern

Single Slit Diffraction: Photon Picture

- In small angle approximation $\sin\theta = \frac{\lambda}{a} \Rightarrow \theta = \frac{\lambda}{a}$

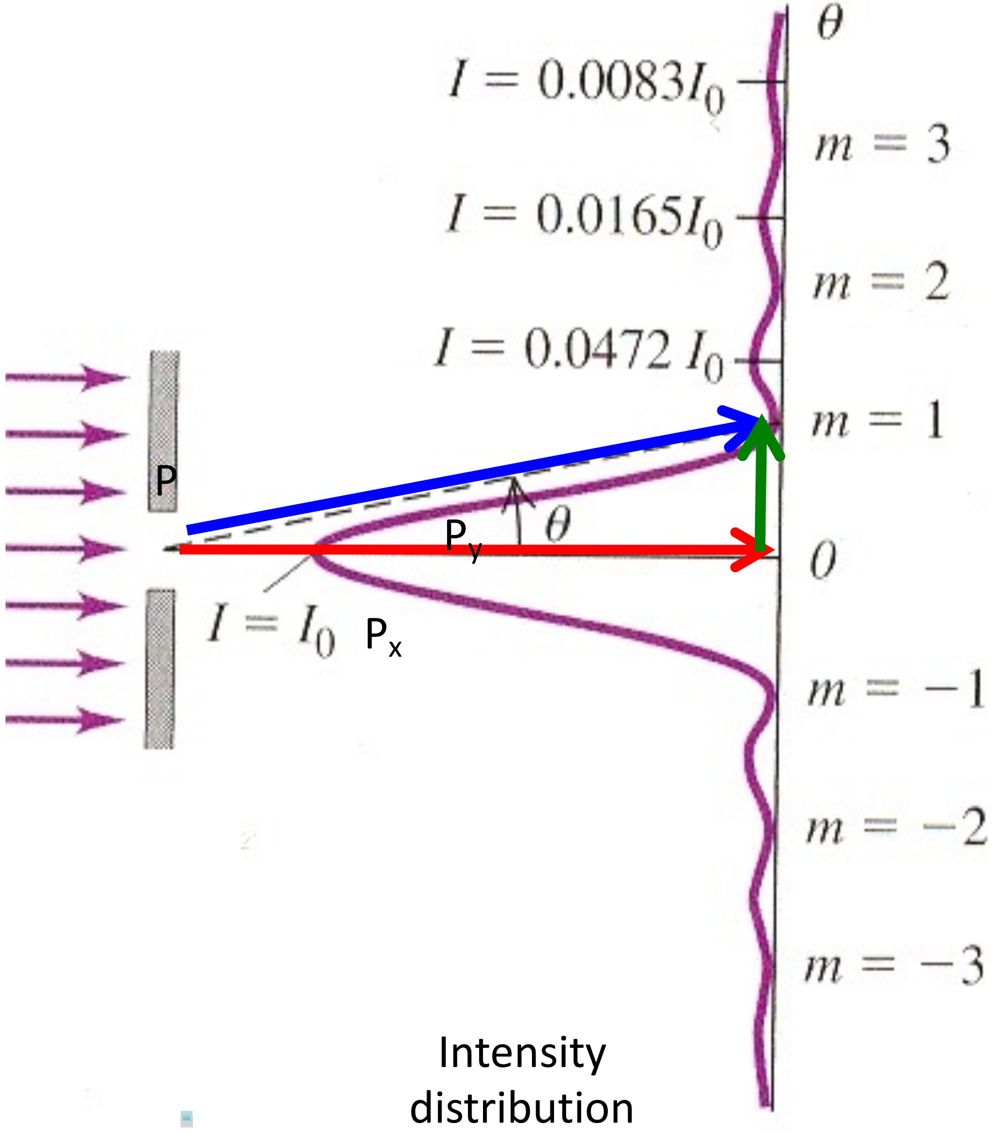
- Photons directed towards outer part of central maximum have momentum

$$\bar{p} = \bar{p}_x + \bar{p}_y$$

$$p_y = \theta p_x = p_x \frac{\lambda}{a} = p_x \frac{h}{p_x a} = \frac{h}{a}$$

- Localizing photons in the y-direction to a slit of width a leads to a spread of y-momenta of at least h/a.

- More we seek to localize a photon (i.e define its position) by shrinking the slit width a the more spread (uncertainty) we induce in its momentum: $\Delta p_y \, \Delta y \sim h$



Intensity distribution

The Uncertainty Principle

Our microscope thought experiments give us an estimate for the uncertainties in position and momentum:

$$\Delta x \Delta p \sim h$$

Heisenberg uncertainty principle states: It is impossible to simultaneously determine the position and momentum of a particle with complete precision.

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

This also means you can’t use classical physics because you can’t specify (exactly) the initial conditions!

Energy Uncertainty

- If we are uncertain of the exact position of a particle, for example an electron somewhere inside an atom, the particle can't have zero kinetic energy.

$$K_{\min} = \frac{p_{\min}{}^2}{2m} \geq \frac{(\Delta p)^2}{2m} \geq \frac{\hbar^2}{2m\ell^2}$$

- The energy uncertainty of a Gaussian wave packet is

$$\Delta E = h\,\Delta f = h\frac{\Delta\omega}{2\pi} = \hbar\,\Delta\omega$$

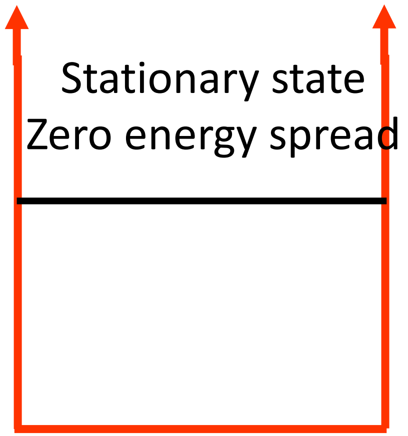
- Combined with the angular frequency relation

$$\Delta\omega\,\Delta t = \frac{\Delta E}{\hbar}\Delta t = \frac{1}{2}$$

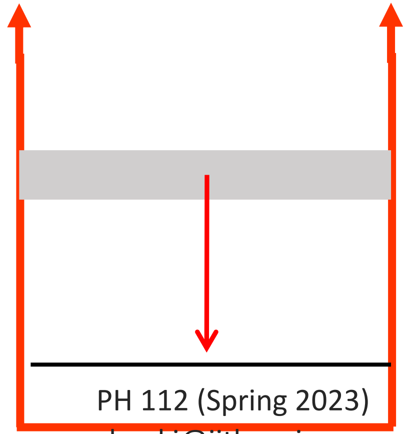
Energy-time Uncertainty

$$\Delta E \Delta t \geq h$$

Uncertainty principle also applies to simultaneous measurements of *energy* and *time*.



The energy can be known with perfect precision ($\Delta E = 0$), only if the measurement is made over an infinite period of time ($\Delta t = \infty$).



The more accurately we know the energy of a body, the less accurately we know how long it possessed that energy!

Decay to lower state with finite lifetime Δt: Energy broadening ΔE (explains, for example "natural linewidth" In atomic spectra)

Summary

- The idea of a perfectly predictable universe cannot be true!

$$\boxed{\Delta x \Delta p \geq \frac{\hbar}{2}}$$

$$\boxed{\Delta E \Delta t \geq h}$$

- There is no such thing as an ideal, objective observer! However nature offers probabilities which can be calculated and tested.

We will soon look at the implications of Uncertainty principle for specific cases.

Recommended Readings

Wave Groups and Dispersion,

section 5.3 in page 164.

Fourier Integral section 5.4