Lecture IV

Last time:
- Heisenberg uncertainty $\Delta x \Delta p_x \geq \frac{\hbar}{2}$
- Diffraction phenomenon

- Fourier decomposition

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

$$= \frac{1}{\sqrt{2\pi t}} \int_{-\infty}^{\infty} dp \, \phi(p) \, e^{ipx+t}$$

$$\phi(p) = \frac{1}{\sqrt{t}} \tilde{\phi}(k)$$

Today:
- How to calculate $\phi(k)$
- Interpretation of $\Psi(x)$ and $\phi(k)$:
  - Probability amplitude & probability density
  - Measurement
The larger \( \Phi(x) \) (or \( \Phi(p) \)), the more the wave function \( \Psi(x) \) resembles the plane wave \( e^{i\lambda x} \) that has definite momentum \( p = \hbar \lambda \), and the more the particle described by the wave function \( \Psi(x) \) is likely to be found to have momentum \( p \), if momentum of the particle were measured.

Conversely, if the particle's momentum is exactly \( p = p_0 = \hbar k_0 \), then the particle's wave function must be \( \Psi(x) = e^{i k_0 x} \), and the particle is equally likely to be found anywhere in space, \( \Delta x \rightarrow \infty \).

To localize a particle in space, we need to add other Fourier components close to \( k_0 \),

\[ \text{constructive interference} \]

\[ k_0 - \Delta k \quad k_0 \quad k_0 + \Delta k \]

\[ \text{destructive interference} \]
To confine a wavefunction to a small region $\Delta x$ of space, one needs many Fourier components, i.e., many plane waves of different momentum $k \in (k_0,k_0+\Delta k)$. We will prove mathematically that, with suitably defined uncertainties $\Delta x, \Delta k$,

\[
\Delta x \cdot \Delta k \geq \frac{1}{2}
\]

follows strictly from Fourier decomposition $\Delta p = \pm \Delta k$.

\[
\Delta x \cdot \Delta p \geq \frac{1}{2}
\]

Heisenberg uncertainty relation.

From this viewpoint, the Heisenberg uncertainty relation follows from the decomposition of a wave into plane waves, i.e., waves with definite wavevector $k$, and the association between wavevector $k$ and momentum $p/k$.

The smaller the region $\Delta x$, the more Fourier components $p/k$ are necessary to produce destructive interference everywhere outside $\Delta x$. 
Corollary: Motion of particles and plane waves from the picture on p. 35 it follows that if you change the relative phase of the different Fourier components, the constructive interference will occur somewhere else in space. This makes sense: we should be able to place a particle at a different location in space while maintaining the momentum distribution.

It follows that if the relative phase between the plane waves changes continuously, the location of constructive interference (i.e., the location of the particle) will move in space.

In terms of wave mechanics, the motion of the particle is simply due to a change of phase between the Fourier components (i.e., the plane waves). Then, to reproduce CM, the Fourier components must rotate their phase in time at a frequency that depends on the momentum p.
Corollary: Time-energy uncertainty

If, instead of Fourier transforming the position coordinate at fixed time \( \psi(x, t_0) \to \phi(u, t_0) \) we fix the position \( x = x_0 \) and study the time variation of the wave function, \( \psi(x_0, t) \)

then we can Fourier decompose the wavefunction into frequency components

\[
\psi(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dw \, \phi(w) e^{-iwt}
\]

Convention: positive frequency \( w \) corresponds to negative phase evolution

Applying the same mathematical and logical arguments as before, we arrive at

\[
\Delta w \Delta t \geq \frac{1}{2} \]

or using the relation between energy and frequency, \( E = \hbar w \),

\[
\Delta E \Delta t \geq \frac{\hbar}{2} \]

time-frequency uncertainty

energy-time Heisenberg uncertainty relation
Probability amplitude and probability density

For light or other waves, the energy per unit volume (or per unit length) is proportional to the square of the (electric) field. Since the number of photons per unit volume is proportional to $|\psi|^2$, we postulate in analogy

$$\left(\text{probability to find a particle between } x \text{ and } x + dx\right) = |\psi(x)|^2 \, dx$$

$|\psi(x)|^2$ is called the probability density (probability per unit length).

The wavefunction $\psi(x)$ is also called the probability amplitude (more exactly: probability density amplitude). In contrast to em fields, $\psi$ is truly a complex quantity.
The requirement that the particle be found somewhere in space leads to the **normalization condition**:

\[ \int_{-\infty}^{\infty} dx \ |\Psi(x)|^2 = 1 \]

In the homework, you will prove **Parseval's theorem**. If \( \tilde{\Phi}(k) = (\Phi(p)) \) is the Fourier transform of a wave function \( \Psi(x) \), i.e.,

\[ \Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \tilde{\Phi}(k) e^{ikx} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dp \Phi(p) e^{ipx/\hbar} \]

then

\[ \int_{-\infty}^{\infty} dx \ |\Psi(x)|^2 = \int_{-\infty}^{\infty} dk \ |\tilde{\Phi}(k)|^2 = \int_{-\infty}^{\infty} dp \ |\Phi(p)|^2 \]

It follows that if the wave function \( \Psi(x) \) is normalized, so is \( \Phi(p) \).

We already argued that if \( \Phi(p) \) is peaked around some value \( p_0 \), the motion of the particle will be similar to that of a classical particle with momentum \( p_0 \) (plane wave \( e^{ipx/\hbar} \)).

Taking into account Parseval's theorem, it is reasonable to interpret \( \Phi(p) \) as the **probability amplitude** for momentum, i.e.
\[
\text{probability to find a particle momentum between } p \text{ and } p + dp \text{ is } 1 \phi(p) dp.
\]

Similarly, \( |\phi(k)|^2 \) is the probability density for the wavevector \( k \).

Note that \( \Delta x \) (or \( \Delta p \)) is not the uncertainty of the measurement device, but associated with the particle itself. If our measurement apparatus can resolve with resolution \( \Delta x_{\text{app}} \ll \Delta x \), and we repeat the experiment with an identically prepared particle many times, we will observe a histogram.

In the limit of a very large number of measurements, the histogram reproduces the probability density \( 1\phi(x)^2 \) or \( 1\phi(p)^2 \).
Note that after measuring a particular value \( x \),
with apparatus uncertainty \( \delta x_{\text{app}} \), the particle is
no longer described by the original wavefunction
\( \psi(x) \), but by a new wavefunction \( \tilde{\psi}(x) \) that
is consistent with the outcome of the measurement
result ("collapse of the wavefunction").

In particular, if \( \delta x_{\text{app}} \ll \delta x \), the spread of the
new wavefunction \( \tilde{\psi}(x) \) in momentum will be
much larger than before, consistent with the
Heisenberg uncertainty relation \( \delta x \cdot \delta p \geq \hbar \)
\[
\delta x \cdot \delta p \geq \delta x_{\text{app}} \cdot \delta p \geq \frac{\hbar}{2}
\]
or
\[
\delta p \geq \frac{\hbar}{2 \delta x_{\text{app}}} \Rightarrow \delta p \geq \frac{\hbar}{2 \delta x} = \delta p
\]

If you now choose to measure momentum with
resolution \( \delta p_{\text{app}} \ll \delta p \), the uncertainty in position
will again increase and so on.
\[ \Phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, \psi(x) e^{-ikx} \]

How to determine the momentum distribution \( |\Phi(p)|^2 \)
given the wavefunction \( \psi(x) \) in position?

The expansion coefficients \( \Phi(k) \) are given by the inverse of the Fourier decomposition:

\[ \Phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, \psi(x) e^{-ikx} \]

Proof:

\[
\frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} dk \, \Phi(k) \, e^{ikx} = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dx' \, \psi(x') \, e^{-ikx'} e^{ikx} \\
= \frac{1}{2\pi} \int_{-\infty}^{\infty} dx' \, \psi(x') \int_{-\infty}^{\infty} dk \, e^{ik(x-x')} \\
\]

What is the value of \( \int_{-\infty}^{\infty} dk \, e^{ik(x-x')} \)?

Qualitatively, if \( x \neq x' \), the integrand oscillates in the complex plane many times as \( k \to \infty \), so the integral is zero. If \( x = x' \), the integral is \( \int_{-\infty}^{\infty} dk \cdot 1 \) and diverges.

So the "function" \( I(y) := \int_{-\infty}^{\infty} dk \, e^{iky} \) looks something
How bad is the divergence? Let us calculate the area under the curve (\(x\) real and positive)

\[
\int_{-\infty}^{\infty} I(y) e^{-xy^2} dy = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{iky} e^{-xy^2} dy dk = \int_{-\infty}^{\infty} \frac{e^{-\frac{1}{4}k^2}}{\sqrt{\pi} \alpha} \]

To calculate the integral we note without proof that

\[
\int_{-\infty}^{\infty} e^{-\alpha(y-\beta)^2} dy = \sqrt{\frac{\pi}{\alpha}}
\]

for any complex \(\alpha, \beta\) with \(\text{Re}(\alpha) \geq 0\)

To bring the above integral into the desired form, we expand the exponent:

\[-xy^2 + iky = -\alpha \left( y^2 - \frac{i}{\alpha} y + \left( \frac{ik}{2\alpha} \right)^2 \right) = -\alpha \left( y - \frac{ik}{2\alpha} \right)^2 - \frac{b^2}{4\alpha}\]

\[
\int_{-\infty}^{\infty} I(y) e^{-xy^2} dy = \int \int \int_{-\infty}^{\infty} e^{-\alpha(y-\frac{ik}{2\alpha})^2 - \frac{b^2}{4\alpha}} dy dk = \int \int e^{-\frac{b^2}{4\alpha}} \sqrt{\frac{\pi}{\alpha}} \sqrt{\frac{\pi}{\alpha}} = 2\pi
\]

independent of the value of \(\alpha\)! Since our probing function \(e^{-xy^2} \rightarrow 1\) as \(y \rightarrow 0\), we conclude that the area under our function \(I(y)\) is finite and
equal to 2π.

We define a "generalized function" (mathematically a distribution) by

\[ \delta(x) := \begin{cases} 0 & \text{for } x \neq 0 \\ \infty & \text{for } x = 0 \end{cases} \]

will the property \( \int_{-\infty}^{\infty} dx \delta(x) = 1 \)

This is the Dirac delta function.

We can think of it as the limiting case of a function of finite width (e.g., a Gaussian or a square function) that is made narrower and narrower, while keeping the area under it constant.

Gaussian \( \delta(x) = \lim_{w \to 0} \frac{1}{\sqrt{2\pi w}} e^{-\frac{x^2}{2w}} \)

We have \( \int_{-\infty}^{\infty} dx \delta(x) = 2\pi \delta(y) \)
Properties of the delta function

What is \( \int_{-\infty}^{\infty} dx \; f(x) \delta(x-x_0) \)? For a function \( f(x) \) that is sufficiently smooth (regular) at \( x = 0 \) and using \( \delta(x-x_0) = 0 \) for \( x \neq x_0 \), we have

\[
\int_{-\infty}^{\infty} dx \; f(x) \delta(x-x_0) = \int_{x_0-\epsilon}^{x_0+\epsilon} dx \; f(x) \delta(x-x_0)
\]

\[
= f(x_0) \int_{x_0-\epsilon}^{x_0+\epsilon} dx \delta(x-x_0) = f(x_0) \int_{-\infty}^{\infty} dx \delta(x) = f(x_0)
\]

Therefore we have

\[
\int_{-\infty}^{\infty} dx \; f(x) \delta(x-x_0) = f(x_0)
\]

Convolution of a function \( f(x) \) with \( \delta(x-x_0) \) "projects out" the value of the function at \( x_0 \).

Without proof we note that

\[
d(x) = \frac{d}{dx} \Theta(x)
\]

The \( \delta \)-function is the derivative of the Heaviside step function.

Derivatives of the delta function can be defined. Integration by parts yields

\[
\int dx \; f(x) \delta'(x-x_0) = -f'(x-x_0)
\]

Convolution with \( \delta' \) projects out the negative derivative at \( x_0 \).