Lecture 7

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February 28, 2016

Contents

1 Wavepackets and Uncertainty

A wavepacket is a superposition of plane waves e^{ikx} with various wavelengths. Let us work with wavepackets at $t = 0$. Such a wavepacket is of the form

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi(k) e^{ikx} dk. \tag{1.1}$$

If we know $\Psi(x,0)$ then $\Phi(k)$ is calculable. In fact, by the Fourier inversion theorem, the function $\Phi(k)$ is the Fourier transform of $\Psi(x,0)$, so we can write

$$\Phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0) e^{-ikx} dx. \tag{1.2}$$

Note the symmetry in the two equations above. Our goal here is to understand how the uncertainties in $\Psi(x,0)$ and $\Phi(k)$ are related. In the quantum mechanical interpretation of the above equations one recalls that a plane wave with momentum $\hbar k$ is of the form e^{ikx}. Thus the Fourier representation of the wave $\Psi(x,0)$ gives the way to represent the wave as a superposition of plane waves of different momenta.

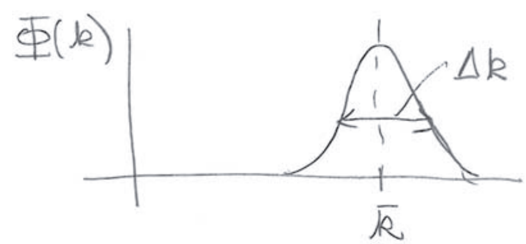

Figure 1: A $\Phi(k)$ that is centered about $k = k_0$ and has width Δk.

Let us consider a positive-definite $\Phi(k)$ that is real, symmetric about a maximum at $k = k_0$, and has a width or uncertainty Δk, as shown in Fig. 1. The resulting wavefunction $\Psi(x,0)$ is centered around $x = 0$. This follows directly from the stationary phase argument applied to (1.1). The wavefunction will have some width Δx, as shown in Fig. 2. Note that we are plotting there the absolute value $|\Psi(x,0)|$ of the wave packet. Since $\Psi(x,0)$ is complex, the other option would have been to plot the real and imaginary parts of $\Psi(x,0)$.

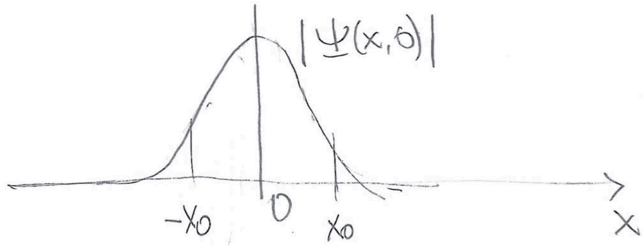

Figure 2: The $\Psi(x,0)$ corresponding to $\Phi(k)$ shown in Fig. 1, centered around $x=0$ with width Δx.

Indeed, in our case $\Psi(x,0)$ is not real! We can show that

$$\boxed{\Psi(x,0) \text{ is real if and only if } \ \Phi^*(-k)=\Phi(k)\,.} \tag{1.3}$$

Begin by complex conjugating the expression (1.1) for $\Psi(x,0)$:

$$\Psi^*(x,0)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Phi^*(k)e^{-ikx}dk \;=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Phi^*(-k)e^{ikx}dk\,. \tag{1.4}$$

In the second step we let $k\to -k$ in the integral, which is allowable because we are integrating over *all* k, and the two sign flips, one from the measure dk and one from switching the limits of integration, cancel each other out. If $\Phi^*(-k)=\Phi(k)$ then

$$\Psi^*(x,0)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Phi(k)e^{ikx}dk=\Psi(x,0), \tag{1.5}$$

as we wanted to check. If, on the other hand we know that $\Psi(x,0)$ is real then the equality of Ψ^* and Ψ gives

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Phi^*(-k)e^{ikx}dk \;=\; \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Phi(k)e^{ikx}dk\,. \tag{1.6}$$

This is equivalent to

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\underbrace{\big(\Phi^*(-k)\;-\;\Phi(k)\big)}\,e^{ikx}dk \;=\; 0\,. \tag{1.7}$$

This equation actually means that the object over the brace must vanish. Indeed, the integral is computing the Fourier transform of the object with the brace, and it tells us that it is zero. But a function with zero Fourier transform must be zero itself (by the Fourier theorem). Therefore reality implies $\Phi^*(-k)=\Phi(k)$, as we wanted to show.

The condition $\Phi^*(-k)=\Phi(k)$ implies that whenever Φ is non-zero for some k it must also be non-zero for $-k$. This is not true for our chosen $\Phi(k)$: there a bump around k_0 but is no corresponding bump around $-k_0$. Therefore $\Psi(x,0)$ is not real and $\Psi(x,0)$ will have both a real and an imaginary part, both centered on $x=0$, as shown in Fig. 3.

Let's now get to the issue of width. Consider the integral for $\Psi(x,0)$

$$\Psi(x,0)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Phi(k)e^{ikx}dk\,, \tag{1.8}$$

and change variable of integration by letting $k=k_0+\widetilde{k}$, where the new variable of integration $\widetilde{k}$ parameterizes distance to the peak in the momentum distribution. We then have

$$\Psi(x,0)=\frac{1}{\sqrt{2\pi}}e^{ik_0x}\int_{-\infty}^{\infty}\Phi\left(k_0+\widetilde{k}\right)e^{i\widetilde{k}x}\,d\widetilde{k}. \tag{1.9}$$

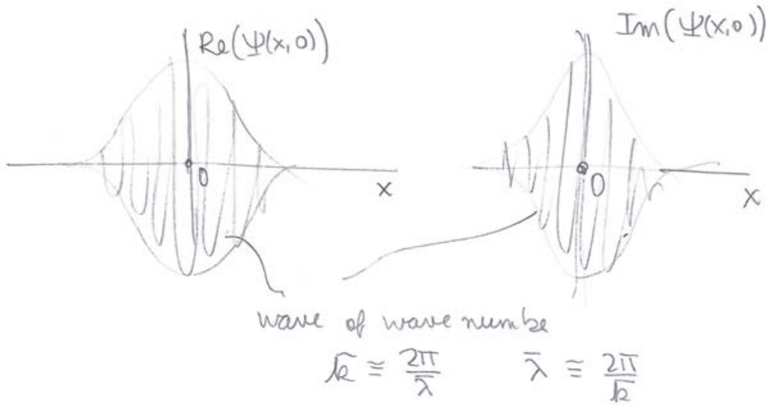

Figure 3: The real and imaginary parts of $\Psi(x,0)$.

As we integrate over $\widetilde{k}$, the most relevant region is

$$\widetilde{k} \in \left[-\tfrac{\Delta k}{2}, \tfrac{\Delta k}{2}\right] , \tag{1.10}$$

because this is where $\Phi(k)$ is large. As we sweep this region, the phase $\widetilde{k}x$ in the exponential varies in the interval

$$\widetilde{k}x \in \left[-\tfrac{\Delta k}{2}x\,,\ \tfrac{\Delta k}{2}x\right] \quad (\text{for } x > 0)\,, \tag{1.11}$$

and the total phase excursion is $\Delta k\, x$. We will get a substantial contribution to the integral for a small total phase excursion; if the excursion is large, the integral will get washed out. Thus, we get a significant contribution for $\Delta k|x| \lesssim 1$, and have cancelling contributions for $\Delta k|x| \gg 1$.

From this, we conclude that $\Psi(x,0)$ will be nonzero for $x \in (-x_0, x_0)$ where x_0 is a constant for which $\Delta k x_0 \approx 1$. We identify the width of $\Psi(x,0)$ with $\Delta x := 2x_0$ and therefore we have $\Delta k\,\frac{1}{2}\Delta x \approx 1$. Since factors of two are clearly unreliable in this argument, we simply record

$$\boxed{\Delta x\, \Delta k \,\approx 1\,.} \tag{1.12}$$

This is what we wanted to show. The product of the uncertainty in the momentum distribution and the uncertainty in the position is a constant of order one. This uncertainty product is not quantum mechanical; as you have seen, it follows from properties of Fourier transforms.

The quantum mechanical input appears when we identify $\hbar k$ as the momentum p. This identification allows us to relate momentum and k uncertainties:

$$\Delta p \;=\; \hbar \Delta k\,. \tag{1.13}$$

As a result, we can multiply equation (1.12) by $\hbar$ to find:

$$\Delta x\, \Delta p \,\approx\, \hbar\,. \tag{1.14}$$

This is the rough version of the Heisenberg uncertainty product. The precise version requires definining Δx and Δp precisely. One can then show that

$$\boxed{\text{Heisenberg uncertainty product:} \quad \Delta x\, \Delta p \,\geq\, \tfrac{\hbar}{2}\,.} \tag{1.15}$$

The product of uncertainties has a lower bound.

Example: Consider the case where $\Phi(k)$ is a finite step of width Δk and height $1/\sqrt{\Delta k}$, as shown in Fig. 4. Find $\Psi(x,t)$ and estimate the value of Δx.

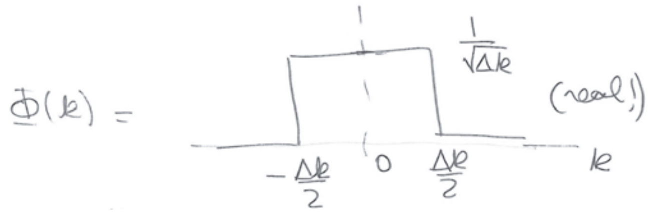

Figure 4: A momentum distribution.

Note that the $\Psi(x,0)$ we aim to calculate should be real because $\Phi^*(-k) = \Phi(k)$. From the integral representation,

$$\begin{aligned}
\Psi(x,0) &= \frac{1}{\sqrt{2\pi}} \int_{-\frac{\Delta k}{2}}^{\frac{\Delta k}{2}} \frac{1}{\sqrt{\Delta k}} e^{ikx} dk \\
&= \frac{1}{\sqrt{2\pi\Delta k}} \left. \frac{e^{ikx}}{ix} \right|_{-\frac{\Delta k}{2}}^{\frac{\Delta k}{2}} \\
&= \frac{1}{\sqrt{2\pi\Delta k}} \frac{e^{i\frac{\Delta k x}{2}} - e^{-i\frac{\Delta k x}{2}}}{ix} \\
&= \frac{1}{\sqrt{2\pi\Delta k}} \, \frac{2}{x} \sin\frac{\Delta k x}{2} \;=\; \sqrt{\frac{\Delta k}{2\pi}} \, \frac{\sin\frac{\Delta k x}{2}}{\frac{\Delta k x}{2}} \,.
\end{aligned} \tag{1.16}$$

We display $\Psi(x,0)$ in Fig. 5. We estimate

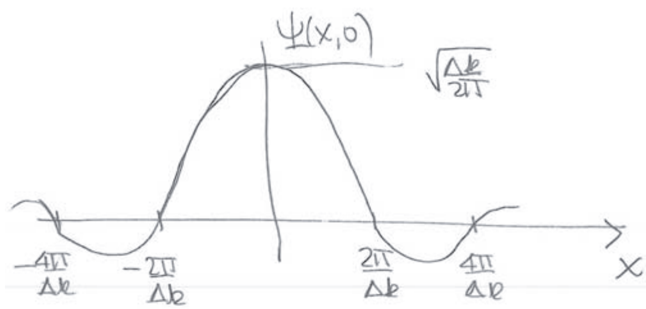

Figure 5: The $\Psi(x,0)$ corresponding to $\Phi(k)$.

$$\Delta x \approx \frac{2\pi}{\Delta k} \quad \rightarrow \quad \Delta x \Delta k \approx 2\pi \,. \tag{1.17}$$

2 Wavepacket Shape Changes

In order to appreciate general features of the motion of a wave-packet we looked at the general solution of the Schrödinger equation

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi(k) e^{i(kx - \omega(k)t)} dk \,, \tag{2.18}$$

and under the assumption that $\Phi(k)$ peaks around some value $k = k_0$ we expanded the frequency $\omega(k)$ in a Taylor expansion around $k = k_0$. Keeping terms up to and including $(k - k_0)^2$ we have

$$\omega(k) = \omega(k_0) + (k - k_0)\, \frac{d\omega}{dk}\bigg|_{k_0} + \frac{1}{2}(k - k_0)^2\, \frac{d^2\omega}{dk^2}\bigg|_{k_0} . \tag{2.19}$$

The second term played a role in the determination of the group velocity and the next term, with second derivatives of ω is responsible for the shape distorsion that occurs as time goes by. The derivatives are promptly evaluated,

$$\frac{d\omega}{dk} = \frac{dE}{dp} = \frac{p}{m} = \frac{\hbar k}{m}, \qquad \frac{d^2\omega}{dk^2} = \frac{\hbar}{m} . \tag{2.20}$$

Since all higher derivatives vanish, the expansion in (2.19) is actually exact as written. What kind of phase contribution are we neglecting when we ignore the last term in (2.19)? We have

$$e^{-i\omega(k)t} = e^{\cdots\; -i\frac{1}{2}(k-k_0)^2 \frac{\hbar}{m} t} . \tag{2.21}$$

Assume we start with the packet at $t = 0$ and evolve in time to $t > 0$. This phase will be ignorable as long as its magnitude is significantly less than one:

$$(k - k_0)^2 \frac{\hbar}{m} t \;\ll\; 1. \tag{2.22}$$

We can estimate $(k - k_0)^2 \approx (\Delta k)^2$ since the relevant k values must be within the width of the momentum distribution. Moreover since $\Delta p = \hbar \Delta k$ we get

$$\frac{(\Delta p)^2 t}{m\hbar} \;\ll\; 1. \tag{2.23}$$

Thus, the condition for minimal shape change is

$$\boxed{\; t \;\ll\; \frac{m\hbar}{(\Delta p)^2} . \;} \tag{2.24}$$

We can express the inequality in terms of position uncertainty using $\Delta x \Delta p \approx \hbar$. We then get

$$\boxed{\; t \;\ll\; \frac{m}{\hbar}(\Delta x)^2 . \;} \tag{2.25}$$

Also from (2.24) we can write

$$\frac{\Delta p\, t}{m} \;\ll\; \frac{\hbar}{\Delta p} , \tag{2.26}$$

which gives

$$\boxed{\; \frac{\Delta p}{m} t \;\ll\; \Delta x . \;} \tag{2.27}$$

This inequality has a clear interpretation. First note that $\Delta p/m$ represents the uncertainty in the velocity of the packet. There will be shape change when this velocity uncertainty through time produces position uncertainties comparable to the width Δx of the wave packet.

In all of the above inequalities we use $\ll$ and this gives the condition for *negligible* shape change. If we replace $\ll$ by $\approx$ we are giving an estimate for some *measurable* change in shape.

Exercise: Assume we have localized an electron down to $\Delta x = 10^{-10}$m. Estimate the maximum time t that it may remain localized to that level.

Using (2.25) we have

$$t \approx \frac{m(\Delta x)^2}{\hbar} = \frac{mc^2(\Delta x)^2}{\hbar c \cdot c} = \frac{0.5\,\text{MeV} \cdot 10^{-20}\text{m}^2}{200\,\text{MeVfm} \cdot 3 \times 10^8\text{m/s}} \approx 10^{-16}\text{s}. \tag{2.28}$$

If we originally had $\Delta x = 10^{-2}$m, we would have gotten $t \approx 1$s!

3 Time evolution of a free wave packet

Suppose you know the wavefunction $\Psi(x,0)$ at time equal zero. Your goal is finding $\Psi(x,t)$. This is accomplished in a few simple steps.

1. Use $\Psi(x,0)$ to compute $\Phi(k)$:

$$\Phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, \Psi(x,0) e^{-ikx}\,. \tag{3.1}$$

2. Use $\Phi(k)$ to rewrite $\Psi(x,0)$ as a superposition of plane waves:

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi(k) e^{ikx} dk\,. \tag{3.2}$$

   This is useful because we know how plane waves evolve in time. The above is called the Fourier representation of $\Psi(x,0)$.

3. A plane wave $\psi_k(x,0) = e^{ikx}$ evolves in time into $\psi_k(x,t) = e^{i(kx-\omega(k)t)}$ with $\hbar\omega = \frac{\hbar^2 k^2}{2m}$. Using superposition we have that (3.2) evolves into

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi(k) e^{i(kx-\omega(k)t)} dk. \tag{3.3}$$

   This is in fact the answer for $\Psi(x,t)$. One can easily confirm this is the solution because: (i) it solves the Schrödinger equation (check that!) and (ii) setting $t = 0$ in $\Psi(x,t)$ gives us the initial wavefunction (3.2) that represented the initial condition.

4. If possible, do the integral over k to find a closed form expression for $\Psi(x,t)$. If too hard, the integral can always be done numerically.

Example: Evolution of a free Gaussian wave packet. Take

$$\psi_a(x,0) = \frac{1}{(2\pi)^{1/4}\sqrt{a}}\, e^{-x^2/4a^2}. \tag{3.4}$$

This is a gaussian wave packet at $t = 0$. The constant a has units of length and $\Delta x \approx a$. The state ψ_a is properly normalized, as you can check that $\int dx |\psi_a(x,0)|^2 = 1$.

We will not do the calculations here, but we can imagine that this packet will change shape as time evolves. What is the time scale τ for shape changes? Equation (2.25) gives us a clue. The right hand side represents a time scale for change of shape. So we must have

$$\tau \;\approx\; \frac{m}{\hbar}a^2\,. \tag{3.5}$$

This is in fact right. You will discover when evolving the Gaussian that the relevant time interval is actually just twice the above time:

$$\tau \;\equiv\; \frac{2ma^2}{\hbar}\,. \tag{3.6}$$

If we consider the norm-squared of the wavefunction

$$|\Psi_a^*(x,0)|^2 \;=\; \frac{1}{\sqrt{2\pi}}\frac{1}{a}e^{-x^2/2a^2}\,, \tag{3.7}$$

you will find that after time evolution one has

$$|\Psi_a^*(x,t)|^2 \;=\; \frac{1}{\sqrt{2\pi}}\frac{1}{a(t)}e^{-x^2/2a^2(t)}, \tag{3.8}$$

where $a(t)$ is a time-dependent width. The goal of your calculation will be to determine $a(t)$ and to see how τ enters in $a(t)$.

Andrew Turner transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.

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Spring 2016

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