Ph195b lecture notes, 1/7/02

Wave Mechanics in one dimension

In this part of the course we'll move on from finite-dimensional quantum systems to the motion of a point particle in one *kinetic* dimension. What we mean by "one dimension" here is that the particle is constrained to move along a line, as opposed to being free to move throughout three-space. Classically we would describe its position by a single variable x, as opposed to a position vector $\vec{r} = (x, y, z)$.

As we are about to see, in quantum mechanics the state of a point particle even in one kinetic dimension corresponds to a vector in an ***infinite-dimensional*** complex Hilbert space.

Quantum Mechanics in Infinite Dimensions

Formally, we may represent the motional state of a point particle (in one kinetic dimension) by a ket in an infinite-dimensional Hilbert space,

$$|\Psi\rangle \in H_\infty.$$

One way to understand the need for an infinite-dimensional Hilbert space is to think about what should constitute a complete (standard) measurement. If this is truly a point particle, then every possible value of position x should correspond to an orthogonal projection operator, or equivalently to one member of a complete orthogonal basis set for the Hilbert space. Since x is a continuous variable, the Hilbert space must be infinite dimensional!

Using $|x\rangle$ to denote the basis ket corresponding to a particular value of position, we find that it should take an infinite number of complex coefficients to fully specify an arbitrary ket $|\Psi\rangle \in H_\infty$:

$$\langle x|\Psi\rangle = \psi(x),$$

where the continuous function $\psi(x)$ here is known as the ***wave function*** corresponding to the state $|\Psi\rangle$. Just as we often used vector representations for bras and kets in finite dimensions, we will almost always use $\psi(x)$ to perform computations in infinite dimensions.

Note that

$$\langle\Psi|x\rangle = \langle x|\Psi\rangle^\dagger = \psi^*(x),$$

and here in infinite dimensions we must replace the usual type of closure relation

$$\sum_{j=1}^{N} |j\rangle\langle j| = \mathbf{1}$$

with an integral

$$\int_{-\infty}^{\infty} dx |x\rangle\langle x| = \mathbf{1}.$$

Hence

$$\langle\Psi_1|\Psi_2\rangle = \langle\Psi_1|\left(\int_{-\infty}^{\infty} dx|x\rangle\langle x|\right)|\Psi_2\rangle$$
$$= \int_{-\infty}^{\infty} dx\langle\Psi_1|x\rangle\langle x|\Psi_2\rangle$$
$$= \int_{-\infty}^{\infty} dx\psi_1^*(x)\psi_2(x)$$

and the norm of a state is

$$\langle\Psi|\Psi\rangle = \int_{-\infty}^{\infty} dx|\psi(x)|^2.$$

We would like to require this to be equal to one for valid quantum states, but below we'll see that this is not always possible. The notion of orthogonality is now

$$\langle\Psi_1|\Psi_2\rangle = \int_{-\infty}^{\infty} dx\psi_1^*(x)\psi_2(x) = 0,$$

which we can compare with finite-dimensional expressions like

$$\sum_j c_j^* d_j = 0$$

where

$$|\Psi_1\rangle = \sum_j c_j|j\rangle, \quad |\Psi_2\rangle = \sum_j d_j|j\rangle.$$

Note also that if we really want to have $\langle x|\Psi\rangle = \psi(x)$, we are forced to conclude that the wave function corresponding to a position basis ket $|x\rangle$ is the singular object

$$|x'\rangle \leftrightarrow \delta(x-x'),$$

so that

$$\langle x'|\Psi\rangle = \int_{-\infty}^{\infty} dx\delta(x-x')\psi(x) = \psi(x'),$$
$$\langle\Psi|x'\rangle = \int_{-\infty}^{\infty} dx\psi^*(x)\delta(x-x') = \psi^*(x').$$

It's not exactly clear what we would mean by the requirement

$$\langle x'|x'\rangle = \int_{-\infty}^{\infty} dx\delta(x-x')\delta(x-x') = 1,$$

so we already have our first instance of a "wave function" we'd like to make use of but is not square-normalizable.

The outer product $|\Psi\rangle\langle\Psi|$ of a state with itself is still an operator, with matrix elements

$$\langle x'|(|\Psi\rangle\langle\Psi|)|x\rangle = \langle x'|\Psi\rangle\langle\Psi|x\rangle$$
$$= \psi(x')\psi^*(x).$$

The most important new subtlety that arises in the interpretation of $|\Psi\rangle$ is that

$$\langle\Psi|\mathbf{\Pi}_x|\Psi\rangle = |\langle x|\Psi\rangle|^2 = |\psi(x)|^2$$

must be interpreted not as the probability to find the particle precisely at position x, but rather as a probability density in the vicinity of position x. Hence, we should think of

$$dP = |\psi(x)|^2 dx$$

as an infinitesimal probability to find the particle within dx of position x, and

$$\Pr(x_1 \le x \le x_2) = \int_{x_1}^{x_2} dx|\psi(x)|^2$$

as the finite probability to find the particle within the interval $x_1 \le x \le x_2$.

Now we are finally ready to introduce the position observable, **x**. We would like this operator to have eigenkets corresponding to the position basis states introduced above,

$$\mathbf{x}|x\rangle = x|x\rangle,$$

Hence the expectation value of position with respect to a given state $|\Psi\rangle$ must be

$$\begin{aligned}\langle\Psi|\mathbf{x}|\Psi\rangle &= \int_{-\infty}^{+\infty} dx\,\langle\Psi|x\rangle\langle x|\Psi\rangle x \\ &= \int_{-\infty}^{+\infty} dx\,\psi^*(x)\,x\,\psi(x),\end{aligned}$$

where in the first line we inserted a spectral decomposition

$$\mathbf{x} = \int_{-\infty}^{+\infty} dx|x\rangle\langle x|\,x.$$

Likewise

$$\langle\Psi|\mathbf{x}^n|\Psi\rangle = \int_{-\infty}^{+\infty} dx\,\psi^*(x)\,x^n\,\psi(x),$$

where our reason for writing x^n between $\psi^*(x)$ and $\psi(x)$ will soon be made clear. Also, although we have assumed here that the operator **x** is an observable, let us defer the details of what it means for an infinite-dimensional operator to be Hermitian.

From classical mechanics we know that a complete kinetic description of particle motion must include momentum as well as position. Thus we have a momentum operator **p**, which we define by its matrix elements

$$\begin{aligned}\langle\Psi_1|\mathbf{p}|\Psi_2\rangle &= \int_{-\infty}^{+\infty} dx\,\psi_1^*(x)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi_2(x) \\ &= -i\hbar\int_{-\infty}^{+\infty} dx\,\psi_1^*(x)\,\frac{\partial\psi_2(x)}{\partial x}.\end{aligned}$$

Hence we make the association

$$\mathbf{p} \leftrightarrow -i\hbar\frac{\partial}{\partial x}$$

when working with wave-functions in one dimension. In a sense we may write the eigenvalue equation

$$\begin{aligned}\mathbf{p}|p\rangle &= p|p\rangle, \\ -i\hbar\frac{\partial}{\partial x}\phi_p(x) &= p\phi_p(x),\end{aligned}$$

which implies

$$\phi_p(x) \propto \exp(+ipx/\hbar).$$

Unfortunately we again find that

$$\langle p|p\rangle \propto \int_{-\infty}^{\infty} dx|\exp(-ipx/\hbar)|^2$$

diverges, so we are unable to enforce normalization of the momentum eigenstates. Nevertheless we shall see that they are quite useful, and pick the simplest convention of setting the constant of proportionality to one, so that

$$\langle x|p\rangle = \exp(+ipx/\hbar).$$

Here we should recognize that the wave functions (position representations) corresponding to momentum eigenstates themselves constitute a basis for the space of wave functions – the Fourier basis! In particular, if we have a given wave-function $\psi(x)$ we know there is a function

$$\begin{aligned} \bar{\psi}(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx \exp(-ipx/\hbar)\,\psi(x), \\ \psi(x) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp \exp(+ipx/\hbar)\,\bar{\psi}(p). \end{aligned}$$

In more familiar terminology, if $\psi(x)$ is the "vector" representation of a state $|\Psi\rangle$ in the position basis then $\bar{\psi}(p)$ is its representation in the momentum basis: $\langle p|\Psi\rangle = \bar{\psi}(p)$. The advantage of knowing $\bar{\psi}(p)$ is that the action of the momentum operator is especially easy to express in this basis, *e.g.*,

$$\begin{aligned} \langle\Psi_1|\mathbf{p}|\Psi_2\rangle &= \int_{-\infty}^{\infty} dp \langle\Psi_1|p\rangle\langle p|\Psi_2\rangle p \\ &= \int_{-\infty}^{\infty} dp\, \bar{\psi}_1^*(p)\, p\, \bar{\psi}_2(p), \end{aligned}$$

where again we have used the spectral decomposition

$$\mathbf{p} = \int_{-\infty}^{\infty} dp |p\rangle\langle p| p.$$

Note that we can already derive a commutation relation between the (infinite-dimensional) operators **x** and **p**. Working in position representation,

$$\begin{aligned} \langle\Psi_1|[\mathbf{x},\mathbf{p}]|\Psi_2\rangle &= \langle\Psi_1|\mathbf{xp}|\Psi_2\rangle - \langle\Psi_1|\mathbf{px}|\Psi_2\rangle \\ &= -i\hbar\int_{-\infty}^{\infty} dx \left\{\psi_1^*(x)\, x \frac{\partial}{\partial x}\psi_2(x) - \psi_1^*(x)\frac{\partial}{\partial x} x\psi_2(x)\right\} \\ &= -i\hbar\int_{-\infty}^{\infty} dx \left\{\begin{array}{c} \psi_1^*(x)\, x\frac{\partial}{\partial x}\psi_2(x) \\ -\left(\psi_1^*(x)\psi_2(x) + \psi_1^*(x)\, x\frac{\partial}{\partial x}\psi_2(x)\right) \end{array}\right\} \\ &= i\hbar\int_{-\infty}^{\infty} dx\, \psi_1^*(x)\psi_2(x) \\ &= i\hbar\langle\Psi_1|\Psi_2\rangle. \end{aligned}$$

Since this is true for arbitrary states $|\Psi_1\rangle, |\Psi_2\rangle$ we must have at the operator level

$$[\mathbf{x},\mathbf{p}] = i\hbar\mathbf{1},$$

or simply $[\mathbf{x},\mathbf{p}] = i\hbar$ as it is more commonly written.

Since these two operators have a nonzero commutator, we know that there exists an uncertainty relation

$$\Delta\mathbf{x}\Delta\mathbf{p} \geq \frac{1}{2}|\langle[\mathbf{x},\mathbf{p}]\rangle| = \frac{\hbar}{2}.$$

That is, *there is no state in the state space for which the product of the uncertainties in position and momentum is less than* $\hbar/2$. If we think back for a moment to the general formulation of the Heisenberg Uncertainty Principle,

$$\Delta\mathbf{A}\Delta\mathbf{B} \geq \frac{1}{2}|\langle[\mathbf{A},\mathbf{B}]\rangle|,$$

we noted (for finite dimensions) that the product $\Delta\mathbf{A}\Delta\mathbf{B}$ could at least go to zero for any eigenstate of the operator $[\mathbf{A},\mathbf{B}]$ with eigenvalue zero. In particular, we noted that if **A** and **B** were observables then any eigenstate of **A** or **B** would do the trick, since

$$\begin{aligned}\langle[\mathbf{A},\mathbf{B}]\rangle &= \langle\Psi_A|\mathbf{AB}-\mathbf{BA}|\Psi_A\rangle \\ &= \langle\Psi_A|\mathbf{AB}|\Psi_A\rangle - \langle\Psi_A|\mathbf{BA}|\Psi_A\rangle \\ &= \lambda_A\langle\Psi_A|\mathbf{B}|\Psi_A\rangle - \langle\Psi_A|\mathbf{B}|\Psi_A\rangle\lambda_A \\ &= 0.\end{aligned}$$

In infinite dimensions now, however, this cannot be the case since all the eigenvalues of $[\mathbf{x},\mathbf{p}] = i\hbar\mathbf{1}$ are equal to $i\hbar$! Hence we are somehow forced to conclude that there are ***no*** states in the state space with vanishing uncerainty product – not even position or momentum eigenstates.

To try to see what is going on, let us first think about the uncertainties for a momentum eigenstate. Clearly we have $\Delta\mathbf{p} = 0$, but the wave function for a momentum eigenstate $\langle x|p\rangle = \psi_p(x) = \exp(+ipx/\hbar)$ is as uncertain in position as can be $(\Delta\mathbf{x} \to \infty)$, since $|\psi_p(x)|^2 = 1$ everywhere! Similarly for a position eigenstate $\psi_{x'}(x) = \delta(x-x')$, we have $\Delta\mathbf{x} = 0$ but the Fourier transform gives

$$\begin{aligned}\tilde{\psi}_{x'}(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx\,\exp(-ipx/\hbar)\,\delta(x-x') \\ &= \frac{1}{\sqrt{2\pi\hbar}}\exp(-ipx'/\hbar),\end{aligned}$$

and $|\tilde{\psi}_{x'}(p)|^2$ is a constant for all p. Hence $\Delta\mathbf{p} \to \infty$ for a position eigenstate. One should be careful in thinking about the product of zero and infinity, but what the $\Delta\mathbf{x}\Delta\mathbf{p}$ uncertainty relation really expresses is the following. By adding up Fourier components (momentum eigenstates) we ought to be able to make up wave functions with varying $\Delta\mathbf{x}$ and $\Delta\mathbf{p}$, ranging from delta-functions $\delta(x-x')$ on one extreme to plane waves $\exp(-ipx/\hbar)$ on the other. In between we have things like Gaussian wave functions

$$\psi(x) = \frac{1}{(\pi\sigma_x)^{1/4}}\exp\left(\frac{-x^2}{2\sigma_x}\right),$$

for which

$$\begin{aligned}(\Delta\mathbf{x})^2 &= \frac{1}{\sqrt{\pi\sigma_x}}\int_{-\infty}^{\infty} dx\,\exp\left(\frac{-x^2}{2\sigma_x}\right)x^2\exp\left(\frac{-x^2}{2\sigma_x}\right) \\ &\quad - \left\{\frac{1}{\sqrt{\pi\sigma_x}}\int_{-\infty}^{\infty} dx\,\exp\left(\frac{-x^2}{2\sigma_x}\right)x\exp\left(\frac{-x^2}{2\sigma_x}\right)\right\}^2 \\ &= \frac{1}{\sqrt{\pi\sigma_x}}\int_{-\infty}^{\infty} dx\,x^2\exp\left(\frac{-x^2}{\sigma_x}\right) - \left\{\frac{1}{\sqrt{\pi\sigma_x}}\int_{-\infty}^{\infty} dx\,x\exp\left(\frac{-x^2}{\sigma_x}\right)\right\}^2 \\ &= \frac{1}{\sqrt{\pi\sigma_x}}\frac{\sigma_x\sqrt{\pi\sigma_x}}{2} \\ &= \frac{\sigma_x}{2},\end{aligned}$$

and

$$
\begin{aligned}
(\Delta \mathbf{p})^2 &= \frac{-\hbar^2}{\sqrt{\pi\sigma_x}} \int_{-\infty}^{\infty} dx \exp\left(\frac{-x^2}{2\sigma_x}\right) \frac{\partial^2}{\partial x^2} \exp\left(\frac{-x^2}{2\sigma_x}\right) \\
&\quad - \left\{ \frac{-i\hbar}{\sqrt{\pi\sigma_x}} \int_{-\infty}^{\infty} dx \exp\left(\frac{-x^2}{2\sigma_x}\right) \frac{\partial}{\partial x} \exp\left(\frac{-x^2}{2\sigma_x}\right) \right\}^2 \\
&= \frac{-\hbar^2}{\sqrt{\pi\sigma_x}} \int_{-\infty}^{\infty} dx \exp\left(\frac{-x^2}{2\sigma_x}\right) \frac{\partial}{\partial x} \left[\frac{-x}{\sigma_x} \exp\left(\frac{-x^2}{2\sigma_x}\right) \right] \\
&\quad - \left\{ \frac{-i\hbar}{\sqrt{\pi\sigma_x}} \int_{-\infty}^{\infty} dx \exp\left(\frac{-x^2}{2\sigma_x}\right) \frac{-x}{\sigma_x} \exp\left(\frac{-x^2}{2\sigma_x}\right) \right\}^2 \\
&= \frac{-\hbar^2}{\sqrt{\pi\sigma_x}} \int_{-\infty}^{\infty} dx \exp\left(\frac{-x^2}{2\sigma_x}\right) \left[\frac{-1}{\sigma_x} \exp\left(\frac{-x^2}{2\sigma_x}\right) + \frac{x^2}{\sigma_x^2} \exp\left(\frac{-x^2}{2\sigma_x}\right) \right] \\
&= \frac{\hbar^2}{\sigma_x\sqrt{\pi\sigma_x}} \int_{-\infty}^{\infty} dx \exp\left(\frac{-x^2}{\sigma_x}\right) - \frac{\hbar^2}{\sigma_x^2\sqrt{\pi\sigma_x}} \int_{-\infty}^{\infty} dx\, x^2 \exp\left(\frac{-x^2}{\sigma_x}\right) \\
&= \frac{\hbar^2}{\sigma_x} - \frac{\hbar^2}{\sigma_x^2\sqrt{\pi\sigma_x}} \frac{\sigma_x\sqrt{\pi\sigma_x}}{2} \\
&= \hbar^2\left(\frac{1}{\sigma_x} - \frac{1}{2\sigma_x}\right) \\
&= \frac{\hbar^2}{2\sigma_x}.
\end{aligned}
$$

Hence

$$
\Delta \mathbf{x} \Delta \mathbf{p} = \sqrt{\frac{\sigma_x}{2}\frac{\hbar^2}{2\sigma_x}} = \frac{\hbar}{2}.
$$

As we try to make the Gaussian narrower and narrower in x by reducing σ_x, we see that the width of its Fourier transform grows as $1/\sigma_x$ and in just such a way that the product of uncertainties satisfies the Heisenberg bound! This coordination between $\Delta x \to 0$ and simultaneously $\Delta p \to \infty$ underlies the "wave-particle duality" in quantum mechanics, which we'll discuss further in the next lecture. From one point of view this is some kind of crazy magic in infinite-dimensional Hilbert spaces, but from another it's really just a routine property of Fourier transforms.

We can now write down the Schrödinger Equation for a free particle, where by analogy with classical mechanics we have the free-particle Hamiltonian

$$
\mathbf{H} = \frac{\mathbf{p}^2}{2m}.
$$

Hence

$$
i\hbar\frac{d}{dt}|\Psi(t)\rangle = \frac{\mathbf{p}^2}{2m}|\Psi(t)\rangle,
$$

which we may rewrite as a wave equation by projecting onto the position basis:

$$
\begin{aligned}
i\hbar\frac{d}{dt}\langle x|\Psi(t)\rangle &= \frac{1}{2m}\langle x|\mathbf{p}^2|\Psi(t)\rangle, \\
\frac{\partial}{\partial t}\psi(x,t) &= \frac{i\hbar}{2m}\int_{-\infty}^{\infty} ds\,\delta(s-x)\frac{\partial^2}{\partial s^2}\psi(s,t) \\
\frac{\partial}{\partial t}\psi(x,t) &= \frac{i\hbar}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t).
\end{aligned}
$$

We know from the form of the Hamiltonian that momentum eigenstates should also be stationary states of the Schrödinger Equation, with energy

$$\mathbf{H}|p\rangle = \varepsilon_p|p\rangle, \quad \varepsilon_p = \frac{p^2}{2m}.$$

Indeed from the wave equation we find

$$\begin{aligned}
\frac{\partial}{\partial t}\phi_p(x,t) &= \frac{i\hbar}{2m}\frac{\partial^2}{\partial x^2}\phi_p(x,t) \\
&= \frac{i\hbar}{2m}\frac{\partial^2}{\partial x^2}\phi_p(x,t) \\
&= \frac{i\hbar}{2m}\left(\frac{ip}{\hbar}\right)^2\phi_p(x,t) \\
&= \frac{-ip^2}{2m\hbar}\phi_p(x,t),
\end{aligned}$$

so that

$$\phi_p(x,t) = \exp(-i\varepsilon_p t/\hbar)\exp(ipx/\hbar).$$

Next time we'll look in more detail at the free evolution of various kinds of wave functions.

Wave packets – average motion

Consider a wave packet

$$\begin{aligned}
\psi(x,0) &= \frac{1}{\sqrt{2\pi}}\int dk\,\varphi(k)\exp(ikx), \\
\varphi(k) &= \frac{1}{\sqrt{2\pi}}\int dx\,\psi(x,0)\,\exp(-ikx).
\end{aligned}$$

As we saw for finite-dimensional systems, a good way to propagate the state forward in time is to re-express it in an energy eigenbasis. Then the coefficients just get multiplied by oscillating phase factors,

$$\begin{aligned}
\varphi(k) &\to \varphi(k)\exp(-i\varepsilon_k t/\hbar) \\
&\equiv \varphi(k)\exp(-i\omega_k t).
\end{aligned}$$

Then to get the wave function (in position representation) at time t we just apply an inverse Fourier Transform,

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int dk\,\varphi(k)\exp[i(kx-\omega t)].$$

Consider a "wave packet" for which $\varphi(k)$ is centered around some value k_0 with width Δk. Then we can Taylor expand

$$\omega_k = \omega_{k_0} + (k-k_0)\frac{d}{dk}\omega_k + \cdots$$

Plugging this in we get

$$\psi(x,t) = \exp\left(-i\omega_{k_0} + ik_0\frac{d}{dk}\omega_k\right)\psi\left(x - \frac{d}{dk}\omega_k t, 0\right),$$

so within the limits of validity of the first-order Taylor expansion the wave packet just moves "rigidly."

But what are the limits of validity?

Wave packets – spreading

For the free-particle Schrödinger Equation we have

$$\omega_k = \frac{(\hbar k)^2}{2m}/\hbar$$
$$= \frac{\hbar k^2}{2m},$$

so our Taylor expansion should really be taken to second order (and will then be exact). Then the neglected term in the Taylor expansion is

$$\frac{(k-k_0)^2}{2}\frac{d^2}{dk^2}\omega_k = \frac{\hbar}{2m},$$

so the neglected term in the exponential of the time-evolving wave packet is

$$\frac{\hbar t}{2m} = \frac{(\Delta p)^2}{2m\hbar}t.$$

Evidently we can ignore this as long as it is much smaller than one, implying

$$|t| \ll \frac{m\hbar}{(\Delta p)^2},$$

or (defining $\Delta v = \Delta p/\hbar$)

$$|t|\Delta v \ll \frac{\hbar}{\Delta p} \sim \Delta x.$$

Hence we find that the rigid-motion limit is only good until the intrinsic uncertainty in velocity adds up to a spreading equal to the initial uncertainty in x.