February 11

The Heisenberg Uncertainty Principle

In this lecture, I will discuss the relation between the formalism of the previous lecture and the tactile Schrödinger wavefunctions that we used in the earlier part of the course.

First, though, I would like to make quantitative a qualitative observation from the previous lecture. I showed that, if Hermitian operators A and B commute, action of the operation B does not change the value of A. On the other hand, if A and B do not commute, I claimed that B disturbed the measurement of A. I would now like to prove that, in this latter case, a quantum state cannot at the same time be well defined in A and also well defined in B. To quantify this, choose any state $|v\rangle$. Let

$$\langle A \rangle = \langle v|A|v\rangle \qquad \langle B \rangle = \langle v|B|v\rangle$$

The variance of A in $|v\rangle$ is

$$\sigma_A^2 = \langle v| (A - \langle A\rangle)^2 |v\rangle = \langle v|A^2|v\rangle - \langle A\rangle^2$$

and similarly for B. If $|v\rangle$ is an eigenstate of A, then

$$\langle A\rangle = a_A \qquad \langle A^2\rangle = a_A^2$$

and so

$$\sigma_A^2 = 0$$

Define

$$\bar{A} = A - \langle A \rangle \qquad \bar{B} = B - \langle B \rangle$$

Then I would like to study, for α a real number, the expectation value

$$\langle v | \left(\alpha \bar{A} - \frac{i}{\alpha} \bar{B}\right)\left(\alpha \bar{A} + \frac{i}{\alpha} \bar{B}\right) | v \rangle$$

The value of this expression is positive

$$= \langle \left(\alpha \bar{A} + \frac{i}{\alpha} \bar{B}\right) v \,|\, \left(\alpha \bar{A} + \frac{i}{\alpha} \bar{B}\right) | v \rangle$$

$$= \left\| \left(\alpha \bar{A} + \frac{i}{\alpha} \bar{B}\right) | v \rangle \right\|^2 \geq 0$$

The expression evaluates to

$$\alpha^2 \langle v | \bar{A}^2 | v \rangle + \frac{1}{\alpha^2} \langle v | \bar{B}^2 | v \rangle + i \langle v | [\bar{A}, \bar{B}] | v \rangle$$

Since $\langle A \rangle$, $\langle B \rangle$ are numbers and commute with anything, we can replace

$$[\bar{A}, \bar{B}] = [A, B]$$

Note, also, that

$$-i [A, B]$$

is a Hermitian operator, so its expectation value is a real number. Finally, we have

$$\alpha^2 \sigma_A^2 + \frac{1}{\alpha^2} \sigma_B^2 - \langle v | -i[A,B] | v \rangle \geq 0$$

If we had begun with the same expression with (i/α) replaced by $(-i/\alpha)$, we would have found the same result with a plus sign in front of the last term. Then

$$\alpha^2 \sigma_A^2 + \frac{1}{\alpha^2} \sigma_B^2 \geq \left| \langle v | -i[A,B] | v \rangle \right|$$

Finally, since α can have any value, set

$$\alpha = \frac{\sigma_B}{\sigma_A}$$

This gives, at last, the inequality

$$\sigma_A \sigma_B \geq \frac{1}{2} \left| \langle v | -i[A,B] | v \rangle \right|$$

If $[A, B] \neq 0$, the right-hand side of the inequality is positive. Then, for most states in the Hilbert space, σ_A and σ_B must both be nonzero. If $|v\rangle$ is an eigenstate of A, σ_B must be infinite, that is, the value of B is totally undefined.

Specifically, if $A = X$ and $B = P$, then

$$-i[X,P] = \hbar$$

Then inequality then implies

$$\sigma_x \cdot \sigma_p \geq \frac{1}{2}\hbar$$

This is the *Heisenberg uncertainty principle*. It implies that quantum state of a particle can be well defined both in X and in P.

Macroscopically, the Heisenberg uncertainty principle has no importance. The value of $\hbar$ is extremely small

$$\hbar = 1.05 \times 10^{-34} \text{ J sec}$$

$$\approx (1 \text{ Å}) \cdot (m_e) \cdot (\alpha c)$$

But, for an electron on atomic scales, this effect is of essential importance. In fact, as we will discuss in more detail later, it is this effect that sets the size of the atomic scale.

Now I would like to make more concrete the connection between our abstract Hilbert space formalism and the formalism of Schrödinger wavefunctions. To do this, I will describe in more detail the Hilbert space of complex-valued functions of x

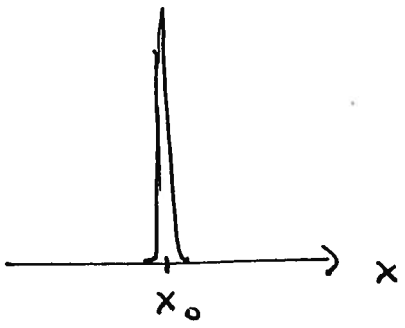
$$f(x)$$

with the norm

$$\langle f | g \rangle = \int_{-\infty}^{\infty} dx \; f^*(x) \, g(x)$$

and boundary conditions such that the operators I discuss are self-adjoint.

An eigenstate of the operator X is a wavefunction extremely highly peaked about some value of x, say x_0



A highly peaked function localized at a point is described by an idealization called the *Dirac delta function*

$$\delta(x-a)$$

The properties of the Dirac delta function are

$$\delta(x-a) = 0 \quad \text{for all } x \neq a$$

$$\int dx\ \delta(x-a)\, f(x) = f(a)$$

for all functions $f(x)$. In particular

$$\int dx\ \delta(x-a) = 1$$

There are many ways to represent the delta function. Here are three useful ones: First, as the limit of a step function,

$$\delta(x) = \lim_{\gamma \to 0} \frac{1}{2\gamma} \cdot \begin{cases} 1 & \text{if } |x| < \gamma \\ 0 & \text{otherwise} \end{cases}$$

second, as the limit of a Gaussian,

$$\delta(x) = \lim_{\sigma \to 0} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2}$$

third, as a limit of a *Lorentzian* function

$$\delta(x) = \lim_{\eta \to 0} \frac{\eta/\pi}{x^2 + \eta^2}$$

All three of these limits arise in physical problems.

Following our earlier rules, the state $|x_0\rangle$ localized at x_0 would be described by a wavefunction normalized to 1. However, it is convenient to adopt a different normalization convention for this case, writing simply

$$\psi_{x_0}(x) = \delta(x - x_0)$$

An excuse for doing things differently here is that the basis of states $|x_0\rangle$ is not only infinite but uncountable. The convention used here will make it easier to sum systematically over all states.

Earlier in the course, I write that any vector in a Hilbert space can be expanded in terms of the eigenvectors of a Hermitian operator. For a discrete spectrum, this relation is represented by the formula

$$|\omega\rangle = \sum_n c_n |v_n\rangle \qquad \text{with} \qquad c_n = \langle v_n | \omega \rangle$$

We can rewrite these equations as

$$|\omega\rangle = \sum_n |v_n\rangle \langle v_n | \omega \rangle$$

or as the representation

$$\underset{\sim}{1} = \sum_n |v_n\rangle\langle v_n|$$

acting on the arbitrary vector $|w\rangle$. This representation of the unit operator is a very useful relation, called the *resolution of the identity.* We can use it to evaluate products of operators, for example

$$\langle u|AB|w\rangle = \sum_n \langle u|A|v_n\rangle\langle v_n|B|w\rangle$$

On a space of functions, the relation reads

$$|f\rangle = \sum_n |\psi_n\rangle\langle\psi_n|f\rangle$$

Writing this out more explicitly,

$$f(x) = \sum_n \psi_n(x) \int dy\, \psi_n^*(y) f(y)$$

This relation is true for all functions in the space. Then we can identify

$$\sum_n \psi_n(x)\psi_n^*(y) = \delta(x-y)$$

since only the delta function satisfies the relation

$$f(x) = \int dy \; \delta(x-y) \, f(y)$$

for any function $f(x)$.

The normalization I have chosen for the wavefunction corresponding to $|x_0\rangle$ leads to a very convenient generalization of this formula to the uncountable basis of X eigenstates. Putting

$$\psi_{x_0}(x) = \delta(x - x_0)$$

and integrating, we find

$$\int dx_0 \; \psi_{x_0}(x) \, \psi^*_{x_0}(y) = \delta(x-y)$$

This is an explicit form of the relation

$$1 = \int_{-\infty}^{\infty} dx_0 \; |x_0\rangle\langle x_0|$$

Also notice that

$$\langle x_0 | \psi \rangle = \int dy \; \psi^*_{x_0}(y) \, \psi(y)$$

evaluates to

$$\int dy \; \delta(y - x_0) \, \psi(y) = \psi(x_0)$$

The inner product of X eigenstates is

$$\langle x_1 | x_2 \rangle = \delta(x_1 - x_2)$$

We can now identify the operator P. The operator P must satisfy the property

$$[X, P] = i\hbar$$

on any function $\psi(x)$. The solution to this constraint is

$$P = -i\hbar \frac{d}{dx}$$

We can check that

$$[X, P]\,\psi(x) = x\left(-i\hbar \frac{d}{dx}\right)\psi(x) - \left(-i\hbar \frac{d}{dx}\right)(x\psi(x))$$

$$= i\hbar\,\psi(x)$$

Now that we have the form of P, we can solve for the eigenstates of P. These satisfy

$$-i\hbar \frac{d}{dx}\,\psi_p(x) = p\,\psi_p(x)$$

The solutions are plane waves

$$\psi_p(x) = e^{i\frac{p}{\hbar}x}$$

It is sometimes more convenient to write these functions as

$$\psi_p(x) = e^{ikx}$$

with the relation $p = \hbar k$. We have now given a formal justification for an ansatz that we used at the beginning of the course. Notice that states of definite P are completely delocalized in X.

I have defined the state $\psi_p(x)$ above in such a way that it is not normalized to 1 but rather has an infinite normalization. Here again, I have made a choice that will be convenient when we sum over this uncountable basis of eigenstates. To repeat,

$$\langle x|p\rangle = \psi_p(x) = e^{i\frac{p}{\hbar}x}$$

The representation

$$P = -i\hbar\frac{d}{dx}$$

gives us a way to write the Hamiltonian of a particle as an operator on wavefunctions. From

$$H = \frac{P^2}{2m} + V(x)$$

we find

$$H\psi(x) = \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi(x)$$

Then the Schrödinger equation, as written in the previous lecture

$$i\hbar \frac{d}{dt} |\psi\rangle = H|\psi\rangle$$

becomes

$$i\hbar \frac{\partial}{\partial t} \psi(x,t) = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x,t)$$

the form of the Schrödinger equation studied in the first lectures of the course.

Any function of x can be expanded in terms of the plane wave eigenstates of P. We are familiar with this on a finite interval, where any function can be expanded as a Fourier series. For functions on the whole real line, the expression of a function in terms of plane waves is called the *Fourier transform.*

We can most easily derive the formulae for the Fourier transform by starting from a finite interval of length L with periodic boundary conditions, and then taking $L \to \infty$. Consider, then, the plane waves on the interval $[0, L]$ satisfying

$$f(x+L) = f(x)$$

These are the functions

$$\psi_n(x) = \frac{1}{\sqrt{L}} e^{i\frac{2\pi n}{L}x}$$

for n an integer which may be positive or negative. I have normalized these functions conventionally,

$$\int_0^L dx \; |\psi_n(x)|^2 = 1$$

The functions are the eigenfunctions of the operator

$$\textcircled{1} = -\frac{d^2}{dx^2}$$

so the Spectral Theorem in the form that I have proved it implies that these functions form a basis for operators on the interval. The resolution of the identity is

$$\sum_n \psi_n(x)\,\psi_n^*(y) = \delta(x-y)$$

or, more explicitly,

$$\sum_n \frac{1}{L}\, e^{i\frac{2\pi n}{L}(x-y)} = \delta(x-y)$$

Now take the limit $L \to \infty$. In this limit, we can replace the sum by an integral. Write

$$k = \frac{2\pi n}{L}$$

and note that

$$\Delta k = \frac{2\pi}{L}\,\Delta n$$

where the interval $\Delta n = 1$. Then

$$\sum_n \;\to\; \int_{-\infty}^{\infty} \frac{L}{2\pi}\, dk$$

The factor L cancels the explicit factor $1/L$, and we find the relation

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} \; e^{ik(x-y)} = \delta(x-y)$$

This equation is another useful representation of the Dirac delta function. If $x = y$, the integral is infinite. If $x \neq y$, the oscillating factors eventually all cancel if we integrate over a large enough interval in k.

Using the normalization of $\psi_p(x)$ given above, we can rewrite this last relation as

$$\int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \; \psi_p(x) \, \psi_p^*(y) = \delta(x-y)$$

In terms of bras and kets, this is

$$\langle x | \int \frac{dp}{2\pi\hbar} \; |p\rangle\langle p| \; |y\rangle = \langle x|y\rangle$$

or

$$\int \frac{dp}{2\pi\hbar} \; |p\rangle\langle p| = \hat{1}$$

The momentum space representation of a wavefunction is

$$\langle p|\psi\rangle = \int_{-\infty}^{\infty} dx \; e^{-i\frac{p}{\hbar}x} \psi(x) = \tilde{\psi}(p)$$

Conversely, we can reconstruct the real space form of a wavefunction by summing over the momentum eigenstates.

$$\langle x|\psi\rangle = \int \frac{dp}{2\pi\hbar} \langle x|p\rangle\langle p|\psi\rangle$$

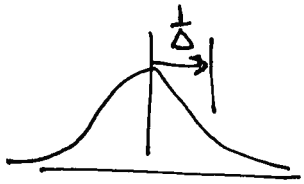
$$= \int \frac{dp}{2\pi\hbar} e^{i\frac{p}{\hbar}x} \tilde{\psi}(p)$$

These two formulae together give the Fourier transform, more conventionally written as

$$f(x) = \int \frac{dk}{2\pi} e^{ikx} \tilde{f}(k) \qquad \tilde{f}(k) = \int dx\, e^{-ikx} f(x)$$

We saw a relation between the real space and momentum space representations of a function in the first lecture of the course. We wrote the momentum space representation

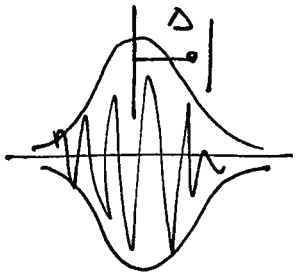
$$\tilde{\psi}(k) = (2\pi\Delta^2)^{\frac{1}{4}} e^{-\frac{\Delta}{2}(k-k_0)^2}$$



and then computed the real space representation

$$\psi(x) = \int \frac{dk}{2\pi} e^{ikx} (2\pi\Delta^2)^{\frac{1}{4}} e^{-\frac{\Delta}{2}(k-k_0)^2}$$

$$= \frac{1}{(2\pi\Delta^2)^{\frac{1}{4}}} e^{-\frac{1}{2\Delta}x^2} e^{ik_0x}$$



We noted a the time that these two Gaussians have an inverse relation in their widths. When $\tilde{\psi}(k)$ is narrow, $\psi(x)$ is wide, and vice versa. Indeed, we can compute the variance of X and P

$$\langle (X-\langle X\rangle)^2\rangle = \int dx\, x^2 |\psi(x)|^2 = \int dx \frac{x^2}{(2\pi\Delta^2)^{\frac{1}{2}}} e^{-\frac{x^2}{\Delta}} = \frac{\Delta^2}{2}$$

$$\langle (P-\langle P\rangle)^2\rangle = \int \frac{dp}{2\pi\hbar} (p-\hbar k_0)^2 |\tilde{\psi}(p)|^2 = \hbar^2 \int \frac{dk}{2\pi} (2\pi\Delta^2)^{\frac{1}{2}} (k-k_0)^2 e^{-\Delta(k-k_0)^2}$$

$$= \frac{\hbar^2}{2\Delta^2}$$

We then find

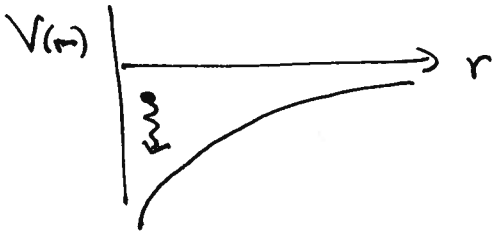
$$\sigma_x = \frac{\Delta}{\sqrt{2}} \qquad \sigma_p = \frac{\hbar}{\sqrt{2}} \frac{1}{\Delta}$$

and so

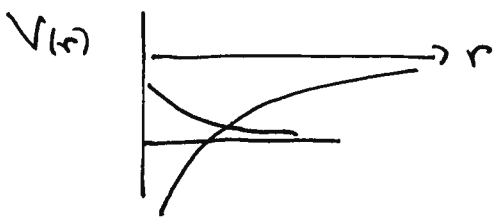
$$\sigma_x \sigma_p = \frac{1}{2} \hbar$$

It seems that this wavefunction precisely saturates the inequality in the Heisenberg uncertainty principle.

The Heisenberg uncertainty principle gives the secret of the stability of the Hydrogen atom. Classically, it is not at all clear that the Hydrogen atom should be stable. A classical particle can take any value of $(\vec{x}, \vec{p})$, so it can fall down toward $\vec{x} = 0$ and have an arbitrarily low energy



In quantum mechanics, this is not possible. A particle cannot be anywhere in phase space; it must be in a state of the Hilbert space of wavefunctions. A wavefunction that is highly localized near $\vec{x} = 0$ has a very large spread of momenta, and so, on average, a very large kinetic energy. We can decrease the kinetic energy by spreading out the function in $\vec{x}$. But then we cannot take advantage of the potential $V(r)$. The best compromise between these positions is the actual 1S state of the Hydrogen atom



which provides the absolute minimum of energy consistent with the principles of quantum mechanics.