C/CS/Phys 191 Uncertainty principle, $\hat{r}$ and $\hat{p}$ in position representation, solving the Schrodinger Eq.

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Fall 2003 Lecture 8

Uncertainty Principle

The uncertainty principle for position and momentum is a consequence of the Fourier transform nature of the relationship between $\mathbf{r}$ and $\mathbf{p}$ representations of the quantum state function $|\psi\rangle$.

Consider a wave packet of plane waves with weight $f(\mathbf{k})$:

$$\begin{aligned}\psi(\mathbf{r},t) &= \int f(\mathbf{k})e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}d\mathbf{k} \\ &= \int A(\mathbf{k})e^{i(\alpha(\mathbf{k})+\mathbf{k}\cdot\mathbf{r}-\omega t)}d\mathbf{k}\end{aligned}$$

where $f(\mathbf{k}) = A(\mathbf{k})e^{i\alpha(\mathbf{k})}$, with A the amplitude and α the phase of the complex function f. This is the integral of an oscillatory function and will be subject to cancellations according to variations of the phase $\phi = \alpha + \mathbf{k}\cdot\mathbf{r} - \omega t$, i.e., there will be interference effects. Constructive interference, resulting in a finite value of the wave function, can be regarded as occurring when the exponential undergoes less than 1 oscillation as $\mathbf{k}$ varies, in the region where $A(\mathbf{k})$ is large.

The change in phase ϕ as we vary, e.g., the x component of $\mathbf{k}$ is

$$\begin{aligned}\Delta\phi_x &\sim \Delta k_x\left(\frac{\partial\phi}{\partial k_x}\right) \\ &= \Delta k_x\left(x - t\frac{\partial\omega}{\partial k_x} + \frac{\partial\alpha}{\partial k_x}\right) \\ &= \Delta k_x\,(x - x_0)\end{aligned}$$

where x_0 is the stationnary phase point that corresponds to the classical motion of the particle represented by the wave packet (Lecture 7). According to our condition above, as long as $\Delta\phi \leq 2\pi$ we will see constructive interference at $\mathbf{r}$ and can detect the particle there. Therefore this requires that $x - x_0 \leq 2\pi/(\Delta k_x)$. Conversely therefore, the end of the wave packet is signalled by the onset of destructive interference which occurs in the regime where

$$x - x_0 = \Delta x \geq 2\pi/(\Delta k_x).$$

So the spatial extent of the wave packet is given by Δx where

$$\Delta x \Delta k_x \geq 2\pi.$$

Using the de Broglie relation $k = p/\hbar$ yields the relation

$$\Delta x \Delta p_x \geq \hbar.$$

This expression tells us that the product of the extent of the wave function in position and momentum representations must be larger than $\hbar$. Similarly you can derive $\Delta y \Delta p_y \geq \hbar$. Note that since there are no cross terms in the derivative of the dot product $\mathbf{k} \cdot \mathbf{r}$ we do not have an analogous relation between e.g., Δx and Δp_y. This relation between the spatial and momentum extent of the wave function is known as the "uncertainty relation". Note carefully what this fundamental relation tells us - we cannot know both the position and its conjugate momentum precisely.

A more precise statement of the uncertainty relation is

$$\Delta x \Delta p_x \geq \hbar/2$$

and is derived in the standard quantum mechanical texts from commutator relations and the Schwarz inequality. Most generally, one finds

$$\Delta A \Delta B \geq \frac{1}{2} |< C >|$$

where $[A, B] = C$. Thus the uncertainty product between expectation values of two operators is related to the commutator of the operators. Two operators that do not commute possess a finite uncertainty product - which tells us we cannot know both expectation values exactly. Recall no simultaneous eigenvalues for non-commuting operators (Lecture 6).

Operators $\hat{p}$ and $\hat{r}$ in position representation

To every obervable physical quantity there corresponds a Hermitian operator (real eigenvalues, orthonormal set of eigenvectors). Thus, we have

$$\hat{\mathbf{p}} = \int d\mathbf{p} |\mathbf{p}\rangle \mathbf{p} \langle \mathbf{p}|.$$

What is the position representation of the momentum operator $\mathbf{p}$? Alternatively, if $\psi(\mathbf{r})$ is the probability amplitude (wave function) for $|\psi\rangle$ in the position representation, what is the corresponding probability amplitude (wave function) for $\hat{\mathbf{p}}|\psi\rangle$?

$$\begin{aligned} \langle \mathbf{r}|\hat{\mathbf{p}}|\mathbf{p}\rangle &= \mathbf{p}\langle \mathbf{r}| |\mathbf{p}\rangle \\ &= \mathbf{p} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}. \end{aligned}$$

Recognize that this is simply the derivative of the exponential, i.e., $\frac{\hbar}{i} \nabla \langle \mathbf{r}| |\mathbf{p}\rangle$. Hence

$$\langle \mathbf{r}|\hat{\mathbf{p}}|\mathbf{p}\rangle = \frac{\boldsymbol{\hbar}}{\mathbf{i}} \nabla \langle \mathbf{r}| |\psi\rangle.$$

Thus $\frac{\hbar}{i} \nabla \psi(\mathbf{r})$ is the action of $\hat{\mathbf{p}}$ on the probability amplitude (wave function) in the position represention, and the momentum operator in the position representation is

$$\hat{\mathbf{p}} = \frac{\hbar}{i} \nabla.$$

Note this is a vector operator, e.g., one component is $\hat{p}_x = \frac{\hbar}{i} \frac{\partial \psi(\mathbf{r})}{\partial x}$. In one dimension we have simply $\hat{p} = \frac{\hbar}{i} \frac{d}{dx}$.

The position operator is simpler. We have

$$\langle \mathbf{r}|\hat{\mathbf{r}}|\psi\rangle = \int d\mathbf{r}' \langle \mathbf{r}||\mathbf{r}'\rangle\langle \mathbf{r}'||\psi\rangle$$
$$= \mathbf{r}\langle \mathbf{r}||\psi\rangle,$$

where we have used the properties of the Dirac delta function (Lecture 7). Thus we have simply

$$\hat{\mathbf{r}}\psi(\mathbf{r}) = \mathbf{r}\psi(\mathbf{r}).$$

You can easily verify by acting sequentially with $\hat{\mathbf{r}}$ on $\psi(\mathbf{r})$, that any function of position, such as r^n, will yield the product $r^n\psi(\mathbf{r})$.

Now we can evaluate the commutator of $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ by looking at the action of this on a wave function, i.e., $[\hat{\mathbf{r}},\hat{\mathbf{p}}]$. You should now be able to show that this commutator is equal to $i\hbar\hat{I}$ where $\hat{I}$ is the identity operator (Problem Set 4).

Solving the Schrodinger Equation

The eigenvalue equation for the Hamiltonian operator,

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

with eigenvalues E_n and corresponding eigenvectors $|\psi_n\rangle$ is often referred to as "the time independent Schrodinger equation". Solutions to this are often also called "stationnary states". Why is this? If you insert one of these eigenvectors into the time-dependent Schrodinger equation, you find the time evolution given simply by a time-dependent phase factor:

$$\begin{aligned} i\hbar\frac{\partial|\psi_n\rangle}{\partial t} &= \hat{H}|\psi_n\rangle \\ &= E_n|\psi_n\rangle, \\ |\psi_n(t)\rangle &= e^{-\frac{i}{\hbar}E_nt}|\psi_n\rangle. \end{aligned}$$

More generally, if $|\psi(0)\rangle = \sum_j a_j(0)|\psi_j\rangle$, we find that the solution to the time-dependent Schrodinger equation is a superposition of contributions each with its own phase factor:

$$|\psi(t)\rangle = \sum_j a_j(0)e^{-\frac{i}{\hbar}E_jt}|\psi_j\rangle.$$

Clearly, knowing $\{E_j\}$ will therefore give us the time evolution. How do we find the eigenvalues E_j? In general they are hard to obtain in a system of interacting particles. So we gain insight from solutions to simple systems that may provide models for more complicated systems, i.e., develop an intuitive understanding. A second route is to develop approximation methods to find solutions. This is the subject of a very broad and powerful approach, but will not be addressed extensively in this course. We shall now examine two simple models that are easily solved and extract some basic features.

Free Particle: solution in position representation

For simplicity, we solve this here in one dimension. Check the solution in higher dimensions as an exercise.

The Hamiltonian is that of a single particle of mass m moving in free space (no potential) on the infinite line.

$$\begin{aligned}
\hat{H} &= \hat{T} + \hat{V} \\
&= \frac{p^2}{2m} + V \\
\hat{V} &= 0 \\
\hat{p} &= \frac{\hbar}{i}\frac{\partial}{\partial x}, \\
\hat{p^2} &= \hat{p}(\hat{p}\psi(x)) \\
&= -\hbar^2 \frac{\partial^2 \psi(x)}{\partial x^2}.
\end{aligned}$$

So we find

$$\begin{aligned}
\hat{H} &= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \\
-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} &= E\psi(x).
\end{aligned}$$

This second order differential equation has two solutions $e^{\pm ikx}$, yielding the general solution

$$\psi(x) = Ae^{ikx} + Be^{-ikx}.$$

This is an energy eigenfunction, i.e., an eigenfunction of $\hat{H}$. The eigenvalue is $E = \hbar^2 k^2/2m$. Note the following features of the solution to this simple model:

- eigenenergies are continuous and not quantized
- eigenergies are doubly degenerate ($\pm k$ both give the same energy), and
- the wave function components $e^{\pm ikx}$ are also eigenfunctions of $\hat{p}$ the momentum operator.

Particle-on-a-ring: solution in position representation

Consider a particle of mass m moving on a circle of constant radius r. The angular coordinate is ϕ and this is periodic, i.e., $\phi + 2\pi \equiv \phi$. You can transform the two dimensional kinetic energy operator $\hat{H} = -\hbar^2/2m(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2})$ from cartesian to angular coordinates r, ϕ ($x = rcos\phi$, $y = rsin\phi$) to obtain

$$\begin{aligned}
\hat{H} &= \hat{T} + \hat{V} \\
&= \frac{p^2}{2I} + V \\
\hat{V} &= 0 \\
\hat{p} &= \frac{\hbar}{i}\frac{\partial}{\partial \phi}, \\
\hat{p^2} &= \hat{p}(\hat{p}\psi(x)) \\
&= -\hbar^2 \frac{\partial^2 \psi(x)}{\partial \phi^2},
\end{aligned}$$

with $I = mr^2$ the moment of inertia. (This plays an analogous role in angular motion to mass in translational motion.) This resembles the time-dependent Schrodinger equation for a free particle and so we expect there will be solutions of the form $e^{\pm ik'\phi}$, where $k' = \pm\sqrt{2IE}/\hbar$. However there is one important difference, namely that the coordinate space is now finite and periodic. In order to ensure that the wave function is single-valued (think, why is this necessary?), we need to impose periodic boundary conditions on $\psi(\phi)$, i.e., $\psi(\phi + 2\pi) = \psi(\phi)$. Hence the allowable solutions are

$$\begin{aligned} \psi_{m_l}(\phi + 2\pi) &= e^{im_l(\phi+2\pi)} \\ &= \psi_{m_l}(\phi)e^{2\pi i m_l} \end{aligned}$$

and to satisfy the periodic boundary conditions we need $e^{2\pi i m_l} = 1 = (-1)^{2m_l}$. This implies that m_l must take the values $0, \pm 1, \pm 2, ...$

To summarize, we have the following features for the particle-on-a-ring:

- energy is quantized, as $E_{m_l} = \frac{\hbar^2 m_l}{2I}$, $m_l = 0, \pm 1, \pm 2, ...$
- doubly degenerate eigenvalues, $\pm|m_l|$
- lowest energy is $E_{m_l} = 0$, $m_l = 0$
- probability amplitude is independent of ϕ - the normalized wave function is $\psi(\phi) = \frac{1}{\sqrt{2\pi}} e^{im_l\phi}$ and so $|\psi(\phi)|^2 = \frac{1}{2\pi}$. m_l and ϕ are complementary observables $\longrightarrow$ the position ϕ is completely uncertain if the quantum number m_l is specified exactly.

What operator is m_l an eigenvalue of? Recall the similarity between the relation between m_l and E, and p and E. Try

$$\begin{aligned} \frac{\hbar}{i}\frac{\partial \psi_{m_l}(\phi)}{\partial \phi} &= \frac{\hbar}{i} i m_l \psi_{m_l}(\phi) \\ &= (m_l\hbar)\psi_{m_l}(\phi). \end{aligned}$$

So $m_l\hbar$ is an eigenvalue of $\frac{\hbar}{i}\frac{\partial}{\partial\phi}$. What is this operator? Recall, in classical mechanics the angular momentum is $\mathbf{L} = \mathbf{r} \times \mathbf{p}$. The z-component of this is $l_z = xp_y - yp_x$ and the corresponding quantum operator is $\hat{l}_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$. Change variables to the angular variables r, ϕ and you will find $\hat{l}_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$. Thus $m_l\hbar$ is an eigenvalue of one component of angular momentum, the single component that results from the angular motion of this particle-on-a-ring.
