Chapter 7 – Uncertainty Principle(s). Measurement in Quantum Mechanics

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Outline

Heisenberg Uncertainty Principle

Heisenberg Uncertainty Principle

Recall the uncertainty principle for classical wave packets

$$\Delta_k \Delta_x \sim 1.$$

The interpretation of this relation is that a narrow packet (the uncertainty in position is small) consists of plane waves with a wide range of wave numbers (the uncertainty in the wave number is large).
Using de Broglie relation $p_x = \hbar k_x$ (consider 1D motion) we obtain

$$\Delta_x \Delta_{p_x} \sim \hbar.$$

or, more precisely,

$$\Delta_x \Delta_{p_x} \geq \frac{\hbar}{2},$$

where Δ_A denotes the standard deviation (uncertainty) a physical quantity A. This inequality is known as the **Heisenberg Uncertainty Principle**.

Illustration. The Gamma-Ray Microscope

Idea: Measure the position of an object (e.g. an electron) by scattering light off it. Measure the position once again a short time later to find the momentum.

Realization: Because of diffraction effects, no lengths smaller than the wavelength of the light used can be measured, therefore use the shortest-wavelength light possible, i.e., gamma rays. The light carries momentum and energy, therefore disturbs the electron in the scattering process, use the minimum intensity possible.

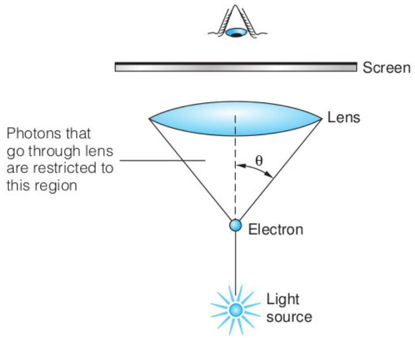
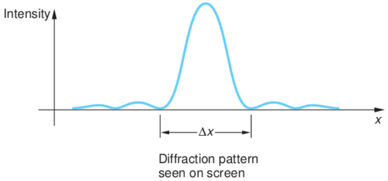
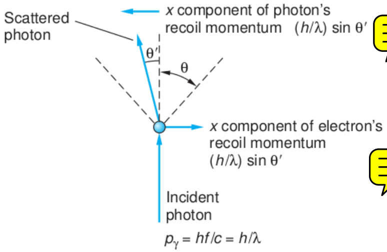


Illustration. The Gamma-Ray Microscope





Uncertainty in the position can be taken as the minimum separation distance, for which two objects can be resolved (recall wave optics) $\Delta_x = \dfrac{\lambda}{2\sin\theta}$.

Assume that the x component of the momentum of the incoming photon is known precisely from the previous measurement. To reach the screen and contribute to the diffraction pattern, the x-component of the scattered photon's momentum needs to be between 0 and $p\sin\theta$.

Illustration. The Gamma-Ray Microscope

By conservation of momentum, the uncertainty in the momentum of the electron after the scattering event must be greater than or equal to that of the scattered photon

$$\Delta_{p_x} \geq p \sin\theta = \frac{h}{\lambda} \sin\theta$$

and hence

$$\Delta_x \cdot \Delta_{p_x} \geq \frac{\lambda}{2\sin\theta} \frac{h}{\lambda} \sin\theta = \frac{h}{2} \geq \frac{\hbar}{2}$$

Conclusion

Even though the electron prior to observation may have had a definite position and momentum, our observation has introduced an uncertainty in the measured values of these quantities. The product of uncertainties cannot be less than the Planck's constant even in an ideal situation.

$$\Delta_x \cdot \Delta_{p_x} \geq \frac{\hbar}{2}$$

Heisenberg Uncertainty Principle

Example 1. Size of the Hydrogen Atom in its ground state

The energy of an electron with momentum p a distance r from a proton is

$$E = \frac{p^2}{2m} - \frac{e^2}{4\pi\varepsilon_0 r}$$

Taking $\Delta_x = r$, we have (the average momentum in the ground state is zero)

$$(\Delta_p)^2 = \langle p^2 \rangle \geq \frac{\hbar^2}{r^2}.$$

The energy is then of the order of

$$E = \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\varepsilon_0 r}.$$

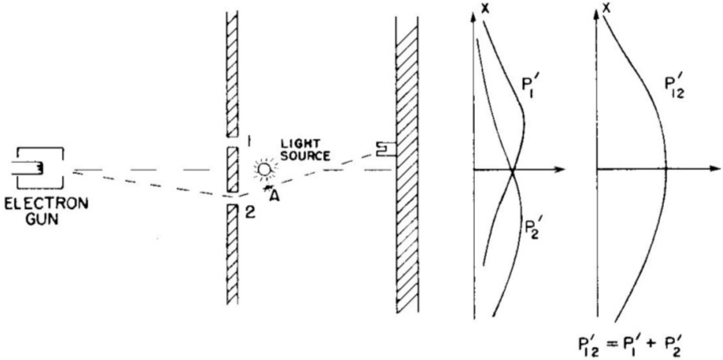
This is a minimum for

$$r = \frac{\hbar^2}{4\pi\varepsilon_0 e^2 m} = a_0,$$

which is the Bohr radius. Hence

$$E(a_0) = -\frac{me^4}{(4\pi\varepsilon_0)^2 2\hbar^2} = -13.6 \text{ eV}$$

Example 2. Disappearing interference pattern in Young's double-slit experiment



If we are able to detect which of the slits the electrons have passed through, the interference pattern disappears.

Measurement in QM is "destructive".

Example 2. Disappearing interference pattern in Young's double-slit experiment

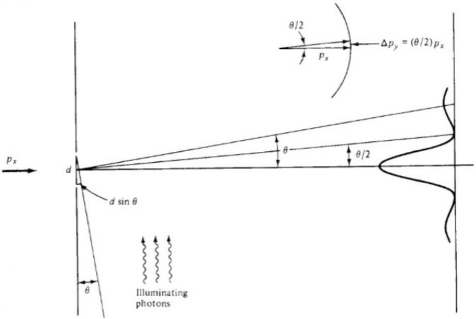


FIGURE 2.16 First maximum at $\theta = 0$; second maximum at $\sin\theta \simeq \theta = \lambda/d$. The angle between the first minimum and the second maximum $= \theta/2 = \lambda/2d$.

If we are able to trace the slit the electron has passed through, then $\Delta_y \ll \frac{d}{2}$. If the interference pattern is not to be destroyed, then the uncertainty in the y-component of electron's momentum $\Delta_{p_y} \ll \frac{\theta}{2} p_x = \frac{h}{2d}$ (scattering cannot displace the electron from the 1st maximum to the 1st minimum). Combining both we get $\Delta_y \Delta_{p_y} \ll \hbar/2$, which **contradicts** the Heisenberg principle!

Uncertainty Principles

Commuting Operators

Commutator

The **commutator** of two operators $\hat{A}, \hat{B}$, denoted[1] as $[\hat{A}, \hat{B}]$, is defined as the operator

$$[\hat{A}, \hat{B}] \stackrel{def}{=} \hat{A}\hat{B} - \hat{B}\hat{A}.$$

Two operators are said to **commute** if and only if $[\hat{A}, \hat{B}] = \hat{0}$ (zero operator).

Physical quantities whose operators commute are called **compatible**.

[1] The commutator is also denoted as $[\hat{A}, \hat{B}]_-$. The sum (again, an operator) $\hat{A}\hat{B} + \hat{B}\hat{A}$ is called the *anticommutator* of operators $\hat{A}, \hat{B}$ and it is denoted as $\{\hat{A}, \hat{B}\}$ or $[\hat{A}, \hat{B}]_+$.

Properties of the Commutator

If $\hat{A}$, $\hat{B}$, and $\hat{C}$ are operators and γ is a (complex) number, then

1. $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$
2. $[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}$
   (similarly with respect to the first argument)
3. $[\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$
   (similarly with respect to the first argument)
4. $[\hat{A}, \gamma] = 0$
5. $[\hat{A}, f(\hat{A})] = 0$,
   where f is any analytic function.

Example: $[\hat{x}, \hat{p}]$

Suppose Ψ is a wave function.

$$[\hat{x}, \hat{p}]\Psi = (\hat{x}\hat{p} - \hat{p}\hat{x})\Psi = [x\left(-i\hbar\frac{\partial \Psi}{\partial x}\right) - \left[-i\hbar\frac{\partial}{\partial x}(x\Psi)\right]$$
$$= i\hbar\left[x\frac{\partial \Psi}{\partial x} + \Psi - x\frac{\partial \Psi}{\partial x}\right] = i\hbar\Psi$$

Hence

$$[\hat{x}, \hat{p}] = i\hbar\hat{I},$$

where $\hat{I}$ is the identity operator[2] (i.e. $\hat{I}\Psi = \Psi$).

Conclusion (important): Position and momentum operators do not commute, i.e. position and momentum are not compatible physical quantities.

[2] From the context it is clear that the rhs is an operator, so the commutator is often simply written as $[\hat{x}, \hat{p}] = i\hbar$, with the identity operator skipped on the rhs.

Schrödinger–Robertson Uncertainty Principle

Schrödinger–Robertson Uncertainty Principle

Consider two physical quantities A and B represented by two operators $\hat{A}$ and $\hat{B}$, respectively, and define two operators

$$\begin{aligned} \tilde{A} &= \hat{A} - \langle A \rangle && (1) \\ \tilde{B} &= \hat{B} - \langle B \rangle . && (2) \end{aligned}$$

Note that these operators are Hermitian (simple exercise). Then the variances of A and B in any quantum state Ψ are[3]

$$\boxed{\begin{aligned} (\Delta_A)^2 &= \langle \Psi, (\tilde{A})^2 \Psi \rangle = \langle \tilde{A}\Psi, \tilde{A}\Psi \rangle = \|\tilde{A}\Psi\|^2 \geq 0 \\ (\Delta_B)^2 &= \langle \Psi, (\tilde{B})^2 \Psi \rangle = \langle \tilde{B}\Psi, \tilde{B}\Psi \rangle = \|\tilde{B}\Psi\|^2 \geq 0. \end{aligned}}$$

Define a quadratic function of a real parameter λ

$$F(\lambda) \stackrel{def}{=} \|(\tilde{A} + i\lambda\tilde{B})\Psi\|^2 .$$

Note that the function is non-negative. Now rewrite F as

[3] Assume that at least one of the inequalities is sharp; in the following discussion we will assume that it is the latter one.

Schrödinger–Robertson Uncertainty Principle

$$
\begin{aligned}
F(\lambda) &= \|(\tilde{A} + i\lambda\tilde{B})\Psi\|^2 \\
&= \langle(\tilde{A} + i\lambda\tilde{B})\Psi, (\tilde{A} + i\lambda\tilde{B})\Psi\rangle \\
&= \langle\Psi, (\tilde{A} - i\lambda\tilde{B})(\tilde{A} + i\lambda\tilde{B})\Psi\rangle \\
&= \langle\Psi, \left(\tilde{A}^2 + \lambda^2\tilde{B}^2 + i\lambda(\tilde{A}\tilde{B} - \tilde{B}\tilde{A})\right)\Psi\rangle \\
&= (\Delta_A)^2 + \lambda^2(\Delta_B)^2 + \lambda\langle\Psi, i[\tilde{A}, \tilde{B}]\Psi\rangle \\
&= \lambda^2(\Delta_B)^2 + \lambda\langle\Psi, i[\hat{A}, \hat{B}]\Psi\rangle + (\Delta_A)^2 \geq 0,
\end{aligned}
$$

where we have used the fact (exercise) that $[\tilde{A}, \tilde{B}] = [\hat{A}, \hat{B}]$. Since $\hat{A}$ and $\hat{B}$ are Hermitian ($\hat{A}^\dagger = \hat{A}$ and $\hat{B}^\dagger = \hat{B}$), then

$$
\left(i[\hat{A}, \hat{B}]\right)^\dagger = -i\left(\hat{A}\hat{B} - \hat{B}\hat{A}\right)^\dagger = -i\left(\hat{B}^\dagger\hat{A}^\dagger - \hat{A}^\dagger\hat{B}^\dagger\right) = i[\hat{A}, \hat{B}],
$$

that is $i[\hat{A}, \hat{B}]$ is Hermitian as well. Hence $\langle\Psi, i[\hat{A}, \hat{B}]\Psi\rangle$ is real[4].

[4] easy exercise (was also shown in one of the previous recitation classes)

Hence the coefficients of the quadratic function

$$F(\lambda) = \lambda^2(\Delta_B)^2 + \lambda\langle\Psi, i[\hat{A}, \hat{B}]\Psi\rangle + (\Delta_A)^2$$

are real and the coefficient next to λ^2 is positive. In order for function F to be non-negative, the discriminant has to be non-positive,i.e.

$$\Big(\langle\Psi, i[\hat{A}, \hat{B}]\Psi\rangle\Big)^2 - 4(\Delta_A)^2(\Delta_B)^2 \leq 0.$$

Schrödinger–Robertson Uncertainty Principle

Hence

$$(\Delta_A)^2(\Delta_B)^2 \geq \frac{1}{4}\left(\langle\Psi, i[\hat{A}, \hat{B}]\Psi\rangle\right)^2$$

or

$$\boxed{\Delta_A\Delta_B \geq \frac{1}{2}\left|\langle\Psi, i[\hat{A}, \hat{B}]\Psi\rangle\right|.}$$

The above inequality is known as the Schrödinger–Robertson uncertainty principle.

Conclusion. If two physical quantities A and B are not compatible (i.e. $[\hat{A}, \hat{B}] \neq \hat{0}$), then the product $\Delta_A\Delta_B$ is bounded from below. That is, the two quantities cannot be simultaneously determined with an arbitrary precision.

Heisenberg Uncertainty Principle

Example: Heisenberg Uncertainty Principle

By taking $\hat{A} = \hat{x}$ and $\hat{B} = \hat{p}$ in the Schrödinger–Robertson uncertainty principle, and recalling that $[\hat{x}, \hat{p}] = i\hbar\hat{I}$, we immediately obtain

$$\Delta_x \Delta_p \geq \frac{\hbar}{2},$$

that is the Heisenberg uncertainty principle.

Comment*. Eigenfunctions of Commuting Operators

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Fact. If two operators $\hat{A}$ and $\hat{B}$ commute, they have common eigenfunctions.

Explanation (case of non-degenerate eigenvalues)

Let ψ_a be an eigenfunction corresponding to a non-degenerate eigenvalue a of an operator $\hat{A}$, i.e.

$$\hat{A}\psi_a = a\psi_a.$$

Since $\hat{A}$ and $\hat{B}$ commute

$$\hat{A}\hat{B}\psi_a = \hat{B}\,\underbrace{\hat{A}\psi_a}_{a\psi_a}.$$

Hence

$$\hat{A}(\hat{B}\psi_a) = a(\hat{B}\psi_a).$$

Since ψ_a is an eigenfunction of the operator $\hat{A}$ corresponding to the eigenvalue a that is non-degenerate, then $\hat{B}\psi_a$ has to be equal to ψ_a up to a multiplicative constant.

Comment*. Eigenfunctions of Commuting Operators

Hence

$$\hat{B}\psi_a = b\psi_a,$$

that is ψ_a is also an eigenfunction of the operator $\hat{B}$ (corresponding to the eigenvalue b).

Conclusion. If $[\hat{A}, \hat{B}] = 0$ and the eigenvalues of $\hat{A}$ are non-degenerate, then every eigenfunction of $\hat{A}$ is also an eigenfunction of $\hat{B}$.

Note.The common eigenfunctions can be then labelled with two eigenvalues, e.g. $\psi_{a,b}$.

Quantum Measurement. Collapse of the Wave Function

Measurement Postulate

Part I. *Suppose that a quantum particle is in a state represented by the wavefunction ψ. For any measurement of a physical quantity A, the only possible outcomes of the measurement are the eigenvalues of the corresponding Hermitian operator $\hat{A}$ representing A.*

Since $\hat{A}$ is Hermitian, ψ can be expanded in eigenfunctions of $\hat{A}$, that is

$$\psi = \sum_n c_n \phi_n$$

where ϕ_n is a normalized eigenfunction of $\hat{A}$ corresponding to the eigenvalue a_n, and $c_n = \langle \phi_n, \psi \rangle$. Since ψ is normalized, then $\sum_n |c_n|^2 = 1$.

What is the interpretation of the coefficients c_n?

Measurement Postulate

Part II. *The probability that the measurement of A yields the value a_n is*

$$\mathrm{Pr}(A = a_n) = |c_n|^2.$$

Please note that this postulate justifies the formula for the average value of a physical quantity in state ψ we have introduced as an axiom before

$$\begin{aligned}
\langle A \rangle &= \langle \psi, \hat{A}\psi \rangle = \langle \sum_n c_n \phi_n, \hat{A} \sum_{n'} c_{n'} \phi_{n'} \rangle \\
&= \sum_n \sum_{n'} c_n^* c_{n'} \langle \phi_n, \underbrace{\hat{A}\phi_{n'}}_{a_{n'}\phi_{n'}} \rangle = \sum_n \sum_{n'} c_n^* c_{n'} a_{n'} \underbrace{\langle \phi_n, \phi_{n'} \rangle}_{\delta_{n,n'}} \\
&= \sum_n a_n |c_n|^2 = \sum_n a_n \cdot \mathrm{Pr}(A = a_n)
\end{aligned}$$

Example

At some instant of time the state of a particle moving in a harmonic potential well $V(x) = m\omega^2 x^2/2$ is described by the (normalized) wave function

$$\psi = \frac{1}{\sqrt{3}}\psi_1 + \sqrt{\frac{2}{3}}\psi_3,$$

where ψ_n is the n-th eigenstate of the Hamiltonian.
The total energy of the particle is measured.

1. What are possible outcomes of the measurement?
2. What is the probability that the measurement yields $\hbar\omega/2$? $3\hbar\omega/2$? $5\hbar\omega/2$?

Wavefunction Collapse

Part III. *Suppose that a measurement of a physical quantity A is performed on a quantum system, yielding the value a. Then the system transfers to the state described the wave function ψ_a, which is the eigenfunction of $\hat{A}$ corresponding to the eigenvalue a.*

This effect is known as the **collapse of the wavefunction**.

Wavefunction Collapse

At some instant of time the state of a particle moving in the harmonic potential well is described by the (normalized) wave function

$$\psi = \frac{1}{\sqrt{3}}\psi_1 + \sqrt{\frac{2}{3}}\psi_3,$$

where ψ_n is the n-th eigenstate of the Hamiltonian.
The total energy of the particle is measured.

1. What is the probability that the measurement yields $3\hbar\omega/2$?
2. What is the probability that the subsequent measurement yields $3\hbar\omega/2$?

Summary: The Postulates of Quantum Mechanics

Postulates of Quantum Mechanics

1. **States**
   The state of a quantum system is represented by a complex-valued function Ψ, called the wavefunction.
2. **Physical Quantities**
   Physical quantities are represented by Hermitian operators. For a particle in a normalized state $\psi = \sum_n c_n \phi_n$, where $\hat{A}\phi_n = a_n \phi_n$, the probability that a measurement of A yields the value a_n is[5]

$$\Pr(A = a_n) = |c_n|^2.$$

[5]Hence, the average value of A in state ψ is $\langle \psi, \hat{A}\psi \rangle$.

Postulates of Quantum Mechanics

3. **Wavefunction Collapse**
   After a measurement of the physical quantity A is performed (yielding the value of a_n) the system transfers to the state represented by the eigenfunction ψ_n of the operator $\hat{A}$, corresponding to the eigenvalue a_n.[6]

4. **Time-Evolution**
   The state of a quantum system, represented by the wavefunction Ψ evolves according to the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi$$

   where $\hat{H}$ is the Hamiltonian of the system, i.e. the operator corresponding to the total energy of the system.

[6] Note that the next measurements of A yield a_n with probability equal to one.