Lecture 24:
The Heisenberg Uncertainty Relation

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Review of Expectation Values and Uncertainty

Recall in Section 4.4, in connection with Postulate 3, we defined the expectation value and uncertainty for a physical observable $\Omega$ because these are the most definite quantities we can calculate given the probabilistic nature of measurement outcomes in quantum mechanics. They are

\[ \langle \Omega \rangle = \langle \psi | \Omega | \psi \rangle = \sum_i P(\omega_i) \omega_i \quad \text{or} \quad \int_{\omega_-}^{\omega_+} d\omega \, P(\omega) \omega \]

\[ \langle (\Delta \Omega)^2 \rangle = \langle \psi | [\Omega - \langle \Omega \rangle]^2 | \psi \rangle = \langle \psi | [\Omega^2 - \langle \Omega \rangle^2] | \psi \rangle = \langle \psi | \Omega^2 | \psi \rangle - \langle \Omega \rangle^2 \]

\[ = \sum_i P(\omega_i) (\omega_i - \langle \Omega \rangle)^2 \quad \text{or} \quad \int_{\omega_-}^{\omega_+} d\omega \, P(\omega) (\omega - \langle \Omega \rangle)^2 \]
Derivation of the Uncertainty Relations

When we consider the uncertainties in two variables, we shall see that the product of their uncertainties has a lower limit that is related to their commutator. This should not surprise as, as we already know that commuting operators are simultaneously diagonalizable and hence can simultaneously have vanishing uncertainties. But now we will generically prove the converse case, in which we consider possibly noncommuting operators.

Consider the commutator of the operators corresponding to two physical variables and write it in the following form:

$$[Ω, Λ] = i Γ$$

If the commutator vanishes, then $Γ$ is the zero operator, the operator that sends every state to the null vector. Because $Ω$ and $Λ$ are Hermitian by assumption, $Γ$ is also Hermitian (which is why the $i$ was introduced).
Now, consider the product of the squares of the uncertainties of the two operators for an arbitrary state $|\psi\rangle$:

$$\langle (\Delta \Omega)^2 \rangle \langle (\Delta \Lambda)^2 \rangle = \langle \psi | \hat{\Omega}^2 | \psi \rangle \langle \psi | \hat{\Lambda}^2 | \psi \rangle \quad \text{with} \quad \tilde{\Omega} = \Omega - \langle \Omega \rangle, \quad \tilde{\Lambda} = \Lambda - \langle \Lambda \rangle$$

$$= (\tilde{\Omega}^\dagger | \psi \rangle \hat{\tilde{\Omega}} | \psi \rangle)^\dagger \tilde{\Lambda} | \psi \rangle$$

$$= (\tilde{\Omega} | \psi \rangle)^\dagger \tilde{\Omega} | \psi \rangle \left(\tilde{\Lambda} | \psi \rangle\right)^\dagger \tilde{\Lambda} | \psi \rangle \quad \text{bec.} \quad \tilde{\Omega}, \tilde{\Lambda} \text{ are Hermitian}$$

$$= |\tilde{\Omega} | \psi \rangle|^2 |\tilde{\Lambda} | \psi \rangle|^2$$

$$\geq \left| (\tilde{\Omega} | \psi \rangle)^\dagger \tilde{\Lambda} | \psi \rangle \right|^2 \quad \text{by Schwarz Inequality, Equation 3.20}$$

$$= \left| \langle \psi | \tilde{\Omega} \tilde{\Lambda} | \psi \rangle \right|^2$$

$$= \left| \langle \psi | \left\{ \frac{1}{2} \left[ \tilde{\Omega} \tilde{\Lambda} + \tilde{\Lambda} \tilde{\Omega} \right] + \frac{1}{2} \left[ \tilde{\Omega} \tilde{\Lambda} - \tilde{\Lambda} \tilde{\Omega} \right] \right\} | \psi \rangle \right|^2$$

$$= \left[ \frac{1}{2} \langle \psi | \left[ \tilde{\Omega}, \tilde{\Lambda} \right] | \psi \rangle + \frac{1}{2} \langle \psi | \left[ \tilde{\Omega}, \tilde{\Lambda} \right] | \psi \rangle \right]^2$$
To evaluate the above, we use the facts that the operator \([\tilde{\Omega}, \tilde{\Lambda}]\) is Hermitian and \([\tilde{\Omega}, \tilde{\Lambda}] = [\Omega, \Lambda] = i \Gamma\) is anti-Hermitian, and so the expectation values \(\langle \psi | [\tilde{\Omega}, \tilde{\Lambda}]_+ | \psi \rangle\) and \(\langle \psi | \Gamma | \psi \rangle\) are perfectly real. The expression above is then of the form \(|a + i b|^2\) where \(a\) and \(b\) are real, so we know the result is \(a^2 + b^2\). We thus have

\[
\langle (\Delta \Omega)^2 \rangle \langle (\Delta \Lambda)^2 \rangle \geq \frac{1}{4} \left[ \langle \psi | [\tilde{\Omega}, \tilde{\Lambda}]_+ | \psi \rangle \right]^2 + \frac{1}{4} \left[ \langle \psi | \Gamma | \psi \rangle \right]^2
\]

This is the generic uncertainty relation. It is not that useful yet because the right side depends on the state \(|\psi\rangle\).

When the commutator is the canonical value \(i \Gamma = i \hbar\), then the above simplifies to

\[
\langle (\Delta \Omega)^2 \rangle \langle (\Delta \Lambda)^2 \rangle \geq \frac{1}{4} \left[ \langle \psi | [\tilde{\Omega}, \tilde{\Lambda}]_+ | \psi \rangle \right]^2 + \frac{\hbar^2}{4}
\]

or

\[
\sqrt{\langle (\Delta \Omega)^2 \rangle} \sqrt{\langle (\Delta \Lambda)^2 \rangle} \geq \frac{\hbar}{2}
\]

where we made the last step because the first term is always nonnegative. This is the Heisenberg uncertainty relation.
Saturation of the Heisenberg Uncertainty Relation

The first condition is

\[ \tilde{\Omega} |\psi\rangle = c \tilde{\Lambda} |\psi\rangle \]

in order that the Schwarz inequality used early in the proof be saturated. Note that we are not requiring the relation \( \tilde{\Omega} = c \tilde{\Lambda} \) to hold in general – then the two would commute and this would all be trivial. We are simply requiring that this hold for the particular state \( |\psi\rangle \) that is going to be a state that saturates the inequality.

The second condition is for the first term in the generic uncertainty relation to vanish:

\[ \langle \psi | \tilde{\Omega}, \tilde{\Lambda} | \psi \rangle = 0 \]

This is obvious, as if this term is nonzero, then it ensures that the relation cannot be an equality.
Example 7.1: The Gaussian Wavefunction

We have twice gone through the demonstration that a state with Gaussian $\{|x\rangle\}$-basis representation always saturates the Heisenberg uncertainty relation for $X$ and $P$, giving

$$\sqrt{\langle (\Delta X)^2 \rangle} \sqrt{\langle (\Delta P)^2 \rangle} = \frac{\hbar}{2}$$

We studied this for both a wave packet propagating freely and for the simple harmonic oscillator. In Section 9.3, Shankar shows explicitly that, for any potential, the Gaussian wavefunction is the only state that renders the inequality an equality by using the first condition above to obtain a differential equation that determines the wavefunction,

$$\left( P - \langle P \rangle \right) |\psi\rangle = c \left( X - \langle X \rangle \right) |\psi\rangle$$

$$\left( -i \hbar \frac{d}{dx} - \langle P \rangle \right) \psi(x) = c \left( x - \langle X \rangle \right) \psi(x)$$

where, in going from the first line to the second, we took the product with $\langle x |$ on the left, inserted completeness in the $\{|x\rangle\}$, and did the completeness integral. The second condition from above is used in Shankar’s proof, too. It is worth going through Shankar’s proof for the sake of the technique.
Example 7.2: Hydrogen Atom

Shankar goes through in detail a calculation of the ground state energy and radius of the hydrogen atom. Again, it is worth studying the technique used, in particular the way in which he approximates the potential term in the Hamiltonian, which is not trivially written as a function of $\langle (\Delta X)^2 \rangle$, and then differentiates $E$ with respect to $\langle (\Delta X)^2 \rangle$ to find the minimum possible energy.
Example 7.3: Diffraction at a Screen

Consider a particle traveling in the $x$ direction with momentum $\hbar k$ incident on a screen with an aperture extending from $y = -a$ to $y = a$. The particle’s position-space wavefunction to the left of the screen is $e^{ikx}$; there is no $y$ dependence. The aperture truncates the wavefunction in $y$ so it vanishes outside the interval $[-a, a]$. The $y$ position uncertainty then becomes $\sqrt{\langle (\Delta Y)^2 \rangle} = \frac{a}{\sqrt{3}}$ (you can check this calculation easily). So the $y$ momentum uncertainty becomes

$$\sqrt{\langle (\Delta P_y)^2 \rangle} \geq \frac{\hbar}{2} \frac{1}{\sqrt{\langle (\Delta Y)^2 \rangle}} = \frac{\hbar \sqrt{3}}{2a}$$

Thus, the propagating plane wave, which initially had no $y$ momentum, acquires a rms $y$ momentum of this size. This causes the wavefunction to spread out in $y$; the angular extent that the image of the particle beam on a far screen will cover is approximately

$$\sqrt{\langle (\Delta \theta)^2 \rangle} = \frac{\sqrt{\langle (\Delta P_y)^2 \rangle}}{\langle P_x \rangle} \geq \frac{\hbar \sqrt{3}}{2a} \frac{1}{\hbar k} = \frac{\sqrt{3}}{2ka}$$
Example 7.4: Size of Nuclei

It is experimentally observed that the binding energy of nuclei is in the few MeV/nucleon range; meaning that nuclei can be caused to break apart by interactions with photons or other particles having this amount of energy. This information can be used to determine the approximate size of a nucleus via simple particle-in-a-box type considerations.

Let $\alpha$ be the typical binding energy per nucleon. Then $\alpha$ is a lower limit on the depth of the potential well, and thus an upper limit on the energy of each nucleon. We may get the momentum uncertainty of a single nucleon from the energy via

$$\frac{\langle (\Delta P)^2 \rangle}{2 m_p} = \alpha \quad \Rightarrow \quad \langle (\Delta P)^2 \rangle = 2 \alpha m_p$$

From this, let’s use the uncertainty principle to determine the position uncertainty

$$\langle (\Delta X)^2 \rangle = \frac{\hbar^2}{4 \frac{1}{\langle (\Delta P)^2 \rangle}} = \frac{\hbar^2}{4} \frac{1}{2 \alpha m_p}$$
Numerically, we have

\[
\sqrt{\langle (\Delta X)^2 \rangle} = \frac{\hbar}{2A \sqrt{2\alpha m_p}}
\]

\[
= \frac{1.0 \times 10^{-34} \text{ J s}}{2 A \sqrt{2\alpha} \times 10^6 \times 1.6 \times 10^{-19} \text{ J} \times 1.7 \times 10^{-27} \text{ kg}}
\]

\[
= \frac{2.1 \times 10^{-15} \text{ m}}{\sqrt{\alpha}}
\]

where we have converted \(\alpha\) to J to do the calculation. For most nuclei, \(\alpha \approx 8 \text{ MeV/nucleon}\), so we get 0.7 fm. Now, this scaling with \(\alpha\) should not necessarily be believed – bigger nuclei have higher binding energies but are also bigger – but the order of magnitude is correct. In practice, nuclei have radii that follow \(r = 1.2 A^{1/3} \text{ fm}\).