Uncertainty principle derivation

Consider a system in a quantum mechanical state \( |\psi\rangle \) and imagine measuring two observables represented by two Hermitian operators \( A \) and \( B \) respectively. For simplicity, we will assume that the spectra of both operators are discrete with

\[
A |a_i\rangle = a_i |a_i\rangle \quad \text{and} \quad B |b_j\rangle = b_j |b_j\rangle .
\]

(1)

Clearly, the measurement of \( A \) yields as the result one of the eigenvalues \( a_i \) and if we expand the state of the system in terms of the eigenkets of \( A \) (these form a complete, orthonormal set) we have

\[
|\psi\rangle = \sum_i \alpha_i |a_i\rangle \quad \text{where} \quad \alpha_i = \langle \psi | a_i \rangle .
\]

(2)

What is the physical interpretation of \( \alpha_i \)?

The results of the measurement of \( A \) yields a distribution of values with the mean given by

\[
\langle A \rangle \equiv \langle \psi | A |\psi\rangle = \sum_i | \alpha_i |^2 a_i .
\]

(3)

Make absolutely certain you can derive the last equality.

Similarly, one can derive \( \langle A^2 \rangle \) and this enables one to define \( \sigma_A^2 \) for this state for the observable \( A \) as usual by

\[
\sigma_A^2 = \langle \psi | A^2 |\psi\rangle - \langle \psi | A |\psi\rangle^2 .
\]

This is defined to be the uncertainty in the measurement of \( A \). We will derive a constraint on the simultaneous measurement of two observables, by computing the uncertainties in measuring \( A \) and \( B \) on the same state \( |\psi\rangle \).

Define

\[
\Delta A = A - < A > \quad \text{and} \quad \Delta B = B - < B >
\]

where \( < A > = \langle \psi | A |\psi\rangle \) as usual. Consider

\[
|\phi\rangle = (\Delta A - i\lambda \Delta B) |\psi\rangle
\]

with real \( \lambda \). Clearly,

\[
\langle \phi | \phi \rangle \geq 0 .
\]

We write this out in detail noting the obvious Hermitian nature of \( \Delta A \) and \( \Delta B \):

\[
\langle \psi | (\Delta A + i\lambda \Delta B)(\Delta A - i\lambda \Delta B) |\psi\rangle \geq 0 .
\]

Since we have

\[
\sigma_A^2 = \langle \psi | (\Delta A)^2 |\psi\rangle \quad \text{and} \quad \sigma_B^2 = \langle \psi | (\Delta B)^2 |\psi\rangle
\]
we obtain the following condition upon substitution
\[ \sigma_A^2 + \lambda^2 \sigma_B^2 - i\lambda \langle \psi \mid [\Delta A, \Delta B] \mid \psi \rangle \geq 0 \]

Note that
\[ [\Delta A, \Delta B] = [A, B] \]
as is clear from the definitions of \( \Delta A \) and \( \Delta B \). Note also that \(-i[A, B]\) is a Hermitian operator\(^1\), call it \( C \); and so \(-i\langle [A, B] \rangle\) is real. We rewrite the earlier result as
\[ \lambda^2 \sigma_B^2 + \lambda \langle C \rangle + \sigma_A^2 \geq 0 . \]

We immediately have the result\(^2\)
\[ \langle C \rangle^2 \leq 4 \sigma_A^2 \sigma_B^2 . \]

Substituting for \( C \) we obtain
\[ \sigma_A^2 \sigma_B^2 \geq \left( \frac{1}{2i} [A, B] \right)^2 . \]

For \( A = x \) and \( B = p_x \) we obtain
\[ \sigma_x \sigma_p \geq \frac{\hbar}{2} \]
one of the standard forms of the Heisenberg uncertainty relation. Note that if two operators commute, for example, \( x \) and \( p_y \), the \( x \)-coordinate and the \( y \)-component of the momentum there are no restrictions on the arbitrarily accurate, simultaneous measurement of the two observables, in principle.

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\(^1\)You should be absolutely clear about this and be able to derive this using the result \((AB)\dagger = B\dagger A\dagger\) and \((cA)\dagger = c^* A\dagger\) for any complex number \( c \).

\(^2\)Given a real quadratic form
\[ ax^2 + bx + c \]
the condition that this is positive definite is obvious from high school algebra. Clearly \( a > 0 \) since the \( ax^2 \) term dominates for large values of \( |x| \). Since we do not want any real roots for the equation
\[ ax^2 + bx + c = 0 \]
(otherwise, between these two roots the function will be negative, just draw a graph) the condition is
\[ b^2 - 4ac < 0 ; \]

Since, \( a > 0 \), this automatically implies \( c > 0 \).
Some remarks: You should be clear that $(\langle \Delta x \rangle^2)$ is not the error in the measurement or related to the resolution of the instrument. It is the intrinsic quantum mechanical spread in the values measured on an ensemble of identically prepared systems. Of course, instrumental resolution is an additional reason for the spread of values that you obtain. We also emphasize that an ensemble measurement is implicit in our derivation and interpretation.

One useful way of understanding the implications is a gedanken experiment in which one measures the position and localizes the particle with a narrow width of $a$ say. The wave function collapses immediately after the measurement. (For simplicity you can imagine this to be a Gaussian of width $a$.) Therefore, the Fourier transform of the wave function that determines the probability of obtaining the momentum to lie between $p$ and $p + dp$ will be broad (proportional to $\hbar/a$) as we discussed earlier. Therefore, an immediate(simultaneous) measurement will not give a precise value of $p$ in an ensemble of identical copies of the system.

The use of the uncertainty principle to estimate energies of bound states:

This is usually not a precise application of the uncertainty principle but amounts to a dimensional argument estimate of the energy. We consider the ground state wave function to have a spatial spread of $a$, i.e., $\langle x^2 \rangle = a^2$, assuming that $\langle x \rangle = 0$. Use the fact that in a bound state $\langle p \rangle = 0$ and therefore, the uncertainty in the momentum, $(\langle \Delta p \rangle^2) = \langle p^2 \rangle$. Then, the minimum value that $\langle p^2 \rangle$ can have is determined by the uncertainty principle. We use this information to estimate the energy for a wave function with this spread and minimize the energy with respect to the spatial width $a$.

Let us do this for the one-dimensional harmonic oscillator. Consider a wave function with width $a$ so that the potential energy is given by

$$\langle V(x) \rangle = \frac{1}{2}m\omega^2\langle x^2 \rangle = \frac{1}{2}m\omega^2a^2$$

where we have used $\langle x \rangle = 0$. The minimum value of $\langle p^2 \rangle$ allowed by the uncertainty principle is $\frac{\hbar^2}{4m^2}$. Thus the energy in this state is given by

$$E(a) = \frac{1}{2}m\omega^2a^2 + \frac{\hbar^2}{8ma^2}.$$  

In the homework problem set you will minimize this and compare with the exact value. Observe that as $a$ increases the potential energy increases and the kinetic energy decreases.

Next consider the hydrogen atom. The Hamiltonian (in three dimensions) is given by

$$H = \frac{\mathbf{p}^2}{2m} - \frac{\mathbf{q}^2}{r}$$

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where $q^2 = \frac{e^2}{4\pi\epsilon_0}$. Consider a wave function with width $a$. We estimate the two terms (roughly) ignoring three dimensionality etc. We have

$$\langle p^2 \rangle \approx \frac{\hbar^2}{a^2}.$$  

How do we estimate the potential energy. Essentially, by dimensional analysis $r$ has units of length and so does $a$. So we set

$$\langle V \rangle = -\frac{q^2}{a}.$$  

Therefore we have

$$E_H(a) = \frac{\hbar^2}{2ma^2} - \frac{q^2}{a}.$$  

Again you will minimize this in the homework and compare with the exact result.