The Uncertainty Principle

Definition of uncertainty:

Consider a system in the state $|\psi\rangle$. We can write $|\psi\rangle$ as a linear combination of a complete set of basis vectors. Let us choose the basis vectors as the orthonormal eigenvectors of a hermitian operator $\hat{A}$ which corresponds to an observable of the system.

Let $|a_i\rangle$, $i = 1, 2, \ldots$, be the eigenvectors of $\hat{A}$ with eigenvalues a_i, i.e.,

$$\hat{A}\,|a_i\rangle = a_i\,|a_i\rangle\,; \quad i = 1, 2, \ldots . \qquad (1)$$

We can now write $|\psi\rangle$ as

$$|\psi\rangle = \sum_i |a_i\rangle\langle a_i|\psi\rangle \quad \ldots\ldots \quad (2)$$

where $\langle a_i|\psi\rangle$ is the 'component' of the state vector $|\psi\rangle$ along the basis vector $|a_i\rangle$.

A measurement of the observable on the system in the state $|\Psi\rangle$ yields one or another eigenvalues a_i of the hermitian operator $\hat{A}$ for which $\langle a_i|\Psi\rangle \neq 0$. The probability for obtaining an eigenvalue a_i is

$$P(a_i) = |\langle a_i|\Psi\rangle|^2 . \quad \cdots\cdots (3)$$

The expectation value of $\hat{A}$ is

$$\langle \hat{A} \rangle \equiv \langle \Psi|\hat{A}|\Psi\rangle . \quad \cdots\cdots (4)$$

<u>Uncertainty of $\hat{A}$</u>

The uncertainty, ΔA, in the measurement of the observable A is defined as

$$(\Delta A)^2 = \sum_i P(a_i)\,(a_i - \langle \hat{A} \rangle)^2 \quad \cdots (5)$$

i.e., the uncertainty is the standard deviation from the mean value of the results obtained in a measurement of the observable A on an ensemble of particles all in the same state $|\Psi\rangle$.

Using Eq. (3) we can write

$$(\Delta A)^2 = \sum_i |\langle a_i|\psi\rangle|^2 (a_i - \langle \hat{A}\rangle)^2$$

$$= \sum_i \langle a_i|\psi\rangle\langle\psi|a_i\rangle (a_i - \langle\hat{A}\rangle)^2$$

$$= \sum_i \langle a_i|\psi\rangle\langle\psi|(\hat{A} - \langle\hat{A}\rangle\hat{\mathbb{1}})^2|a_i\rangle$$

$$= \sum_i \langle\psi|(\hat{A} - \langle\hat{A}\rangle\hat{\mathbb{1}})^2|a_i\rangle\langle a_i|\psi\rangle$$

or,

$$\boxed{(\Delta A)^2 = \langle\psi|(\hat{A} - \langle\hat{A}\rangle\hat{\mathbb{1}})^2|\psi\rangle} \quad \cdots\cdots (5)$$

where we have used the completeness condition of the basis vectors, i.e.,

$$\sum_i |a_i\rangle\langle a_i| = \hat{\mathbb{1}} \quad \cdots\cdots\cdots (6)$$

We can write down an alternative formula for $(\Delta A)^2$ by expanding $(\hat{A} - \langle\hat{A}\rangle\hat{\mathbb{1}})^2$ in Eq. (5).

We have

$$(\Delta A)^2 = \langle\psi|\, \hat{A}^2 - 2\hat{A}\langle\hat{A}\rangle + \langle\hat{A}\rangle^2 \hat{\mathbb{1}} \,|\psi\rangle$$

$$= \langle\psi|\hat{A}^2|\psi\rangle - 2\langle\hat{A}\rangle^2 + \langle\hat{A}\rangle^2$$

or

$$\boxed{\begin{aligned}(\Delta A)^2 &= \langle\psi|\hat{A}^2|\psi\rangle - \langle\hat{A}\rangle^2. \\ &= \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2\end{aligned}} \quad \cdots\cdots (7)$$

We note that the uncertainty, ΔA, of an observable A depends not only on the operator $\hat{A}$ corresponding to the observable but also on the state $|\psi\rangle$ of the system.

As a special case, if the state vector $|\psi\rangle$ of the system is one of the eigenvectors of $\hat{A}$, say $|a_n\rangle$, then

$$P(a_n) = 1$$

and the probability for ~~a~~ obtaining any other eigenvalue is zero.

In such a situation

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle = \langle a_n | \hat{A} | a_n \rangle = a_n$$

and

$$\langle \hat{A}^2 \rangle = a_n^2 .$$

Therefore, from Eq. (7) we see that

$$(\Delta A)^2 = 0$$

i.e.,

$$\Delta A = 0 .$$

Thus, we have shown that

$$\boxed{\text{The uncertainty } \Delta A(\psi) \text{ vanishes when } |\psi\rangle \text{ is an eigenstate of } \hat{A} .}$$

We can give an interesting geometrical interpretation of the uncertainty as follows. Consider the one-dimensional vector subspace U_ψ generated by $|\psi\rangle$. Take the vector $\hat{A}|\psi\rangle$ and project it to the subspace U_ψ. The projection is $\langle\hat{A}\rangle|\psi\rangle$ and the part of $\hat{A}|\psi\rangle$ in the orthogonal subspace $U_\psi^\perp$ is a vector of norm equal to the uncertainty ΔA. Indeed, P_{U_ψ} is

$$P_{U_\psi} = |\psi\rangle\langle\psi| \qquad \text{- - - - - - (8)}$$

so that

$$P_{U_\psi}\hat{A}|\psi\rangle = |\psi\rangle\langle\psi|\hat{A}|\psi\rangle = \langle\hat{A}\rangle|\psi\rangle \qquad \text{---(9)}$$

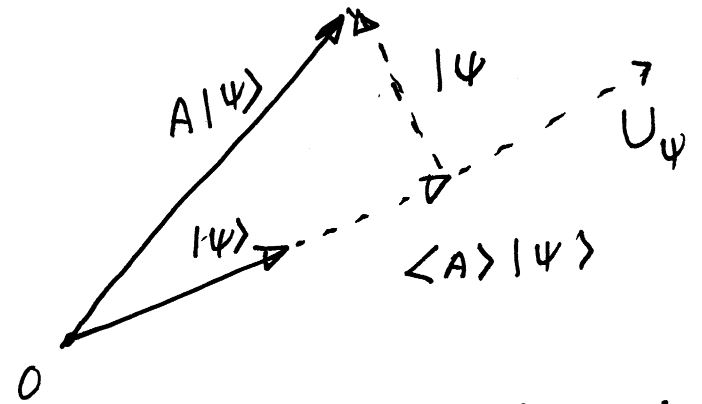


Fig: A state $|\psi\rangle$ and the one-dimensional subspace U_ψ generated by it. The projection of $\hat{A}|\psi\rangle$ on U_ψ is $\langle A\rangle|\psi\rangle$. The orthogonal complement $|\psi_\perp\rangle$ is a vector whose norm is the uncertainty $\Delta A(\psi)$.

Moreover, the vector $\hat{A}|\psi\rangle$ minus its projection must be a vector $|\psi_\perp\rangle$ orthogonal to $|\psi\rangle$:

$$\hat{A}|\psi\rangle - \langle\hat{A}\rangle|\psi\rangle = |\psi_\perp\rangle$$

We can easily confirm that $\langle\psi|\psi_\perp\rangle = 0$.

Now

$$|\psi_\perp\rangle = (\hat{A} - \langle\hat{A}\rangle\hat{\mathbb{1}})|\psi\rangle$$

$$\therefore \| |\psi_\perp\rangle \| = \sqrt{\langle\psi_\perp|\psi_\perp\rangle}$$

$$= \sqrt{\langle\psi|(\hat{A} - \langle\hat{A}\rangle\hat{\mathbb{1}})^2|\psi\rangle}$$

$$= \Delta A. \qquad \cdots\cdots\cdots (10)$$

The Uncertainty Principle

The uncertainty principle is an inequality that is satisfied by the product of the uncertainties of two Hermitian operators that fail to commute. Since the uncertainty of an operator in any given physical state $|\psi\rangle$ of the system is a real number equal to or greater than zero, the product of uncertainties is also a real number equal to or greater than zero. The uncertainty inequality often gives a lower bound for this product.

Derivation of the Uncertainty Principle:

Consider two Hermitian operators $\hat{A}$ and $\hat{B}$ representing two observables of a system. Suppose that the system is in the state $|\psi\rangle$. The uncertainties ΔA and ΔB are given by

$$(\Delta A)^2 = \langle\psi|(\hat{A} - \langle\hat{A}\rangle)^2|\psi\rangle \quad \cdots\cdots (11)$$

and

$$(\Delta B)^2 = \langle\psi|(\hat{B} - \langle\hat{B}\rangle)^2|\psi\rangle, \quad \cdots\cdots (12)$$

The operators $(\hat{A} - \langle\hat{A}\rangle\hat{\mathbb{1}})$ and $(\hat{B} - \langle\hat{B}\rangle\hat{\mathbb{1}})$ are both Hermitian since $\hat{A}$ and $\hat{B}$ are Hermitian,

We now define two kets $|f\rangle$ and $|g\rangle$ as

$$|f\rangle = (\hat{A} - \langle\hat{A}\rangle)|\psi\rangle$$

$$|g\rangle = (\hat{B} - \langle\hat{B}\rangle)|\psi\rangle.$$

The corresponding bras in the dual space are

$$\langle f| = \langle\psi|(\hat{A} - \langle\hat{A}\rangle)$$

$$\langle g| = \langle\psi|(\hat{B} - \langle\hat{B}\rangle).$$

In terms of $|f\rangle$ and $|g\rangle$ we can write

$$(\Delta A)^2(\Delta B)^2 = \langle f|f\rangle\langle g|g\rangle. \quad \cdots\cdots (13)$$

We now use Schwarz inequality

$$\langle f|f\rangle\langle g|g\rangle \geq |\langle f|g\rangle|^2 \quad \text{------(14)}$$

where the equality holds if $|g\rangle \propto |f\rangle$, i.e., if

$$|g\rangle = \lambda|f\rangle \quad \text{.........(15)}$$

with λ equal to a constant which is complex in general.

The uncertainty product (Eq. (13)) can therefore be written as

$$\begin{aligned}(\Delta A)^2(\Delta B)^2 &= \langle f|f\rangle\langle g|g\rangle \\ &\geq |\langle f|g\rangle|^2 \\ &= \left|\langle\Psi|(\hat{A}-\langle\hat{A}\rangle)(\hat{B}-\langle\hat{B}\rangle)|\Psi\rangle\right|^2 \quad \text{..(16)}\end{aligned}$$

where the equality holds if Eq. (15) is satisfied, i.e., if

$$(\hat{B}-\langle\hat{B}\rangle)|\Psi\rangle = \lambda(\hat{A}-\langle\hat{A}\rangle)|\Psi\rangle \quad \text{---(17)}$$

Next, letting

$$\hat{A}' = \hat{A} - \langle \hat{A} \rangle$$

$$\hat{B}' = \hat{B} - \langle \hat{B} \rangle$$

we have

$$(\hat{A} - \langle \hat{A} \rangle)(\hat{B} - \langle \hat{B} \rangle)$$

$$= \hat{A}'\hat{B}'$$

$$= \frac{\hat{A}'\hat{B}' + \hat{B}'\hat{A}'}{2} + \frac{\hat{A}'\hat{B}' - \hat{B}'\hat{A}'}{2}$$

$$= \frac{1}{2}\{\hat{A}', \hat{B}'\} + \frac{1}{2}[\hat{A}', \hat{B}'] \quad \text{------} \quad (18)$$

where

$$\{\hat{A}', \hat{B}'\} = \hat{A}'\hat{B}' + \hat{B}'\hat{A}'$$

is called the anti-commutator of $\hat{A}'$ and $\hat{B}'$. Note that the anti-commutator is a Hermitian operator.

We also note that

$$[\hat{A}', \hat{B}'] = [\hat{A}, \hat{B}] \quad \cdots\cdots (19).$$

The commutator $[\hat{A}, \hat{B}]$ is an anti-Hermitian operator, i.e.,

$$[\hat{A}, \hat{B}]^{\dagger} = -[\hat{A}, \hat{B}].$$

We write $[\hat{A}, \hat{B}]$ as

$$[\hat{A}, \hat{B}] = i\hat{C} \quad \cdots\cdots (20)$$

where $\hat{C}$ is Hermitian.

Now, using Eqs. (18) and (19) in Eq. (16)

we have

$$(\Delta A)^2 (\Delta B)^2 \geq \left| \langle \psi | \hat{A}' \hat{B}' | \psi \rangle \right|^2$$

$$= \left| \frac{1}{2} \langle \psi | \{ \hat{A}', \hat{B}' \} | \psi \rangle + \frac{1}{2} \langle \psi | [\hat{A}, \hat{B}] | \psi \rangle \right|^2.$$

$$\cdots\cdots (21)$$

Since the anticommutator is Hermitian, its expectation value is real. Since the commutator is written as i times a Hermitian operator $\hat{C}$ (Eq. (20)), the expectation value of the commutator is purely imaginary.

Recalling that

$$|a+ib|^2 = a^2+b^2 \quad (a, b \text{ real}),$$

Eq. (21) can be written as

$$(\Delta A)^2(\Delta B)^2 \geq \frac{1}{4}\Big|\underbrace{\langle\psi|\{\hat{A}', \hat{B}'\}|\psi\rangle}_{\text{real}} + i\underbrace{\langle\psi|\hat{C}|\psi\rangle}_{\text{real}}\Big|^2$$

or,

$$(\Delta A)^2(\Delta B)^2 \geq \frac{1}{4}\langle\psi|\{\hat{A}', \hat{B}'\}|\psi\rangle^2 + \frac{1}{4}\langle\psi|\hat{C}|\psi\rangle^2$$

Since $\hat{C} = \frac{1}{i}[\hat{A}, \hat{B}]$, we can also write

$$\boxed{(\Delta A)^2(\Delta B)^2 \geq \underbrace{\langle\psi|\tfrac{1}{2}\{\hat{A}',\hat{B}'\}|\psi\rangle}_{\text{real}}^2 + \underbrace{\langle\psi|\tfrac{1}{2i}[\hat{A},\hat{B}]|\psi\rangle}_{\text{real}}^2} \quad \cdots (22)$$

This can be viewed as the most complete form of the uncertainty inequality. It turns out, however, that the first term on the right hand side is seldom simple enough to be of use, and many times it can be made equal to zero for certain states. At any rate, this term is positive or zero, so it can be dropped while preserving the inequality. This is often done.

Thus we get

$$(\Delta A)^2(\Delta B)^2 \geq \langle\psi|\tfrac{1}{2i}[\hat{A},\hat{B}]|\psi\rangle^2.$$

Taking the square root of this equation and noting that ΔA and ΔB are positive (or zero) we have

$$\boxed{\Delta A\, \Delta B \geq \left| \underbrace{\langle \psi | \frac{1}{2i} [\hat{A}, \hat{B}] | \psi \rangle}_{\text{real}} \right|} \quad \ldots\ldots (23)$$

This is the celebrated Heisenberg uncertainty relation for two Hermitian operators.

We note that the uncertainty product $\Delta A\, \Delta B$ depends, in general, on the operators and the state vector $|\psi\rangle$. Given a state $|\psi\rangle$ we can always calculate the exact values of ΔA and ΔB and hence an exact value for the product $(\Delta A)(\Delta B)$. The uncertainty principle asserts that the value of $\Delta A\, \Delta B$ is greater than or equal to the right hand side of Eq. (23).

The uncertainty principle has the most predictive power about the nature of the physically realizable states when the commutator on the right hand side of Eq. (23) is a c-number, i.e., a multiple of the identity operator. As a very important example, take

$$\hat{A} = \hat{x} \quad \text{and} \quad \hat{B} = \hat{p}_x$$

The commutator of $\hat{x}$ and $\hat{p}_x$ is $i\hbar\hat{\mathbb{1}}$, i.e.,

$$[\hat{x}, p_x] = i\hbar\hat{\mathbb{1}}$$

so that the uncertainty principle for x and p_x is

$$\boxed{\Delta x \, \Delta p_x \geq \frac{\hbar}{2}} \quad \ldots\ldots\ldots (24)$$

This very important uncertainty relation ~~between~~ for $\hat{x}$ and $\hat{p}_x$ states that in all physically realizable states Δx and Δp_x are corelated in such a manner that if Δx is very small in a certain state than Δp_x is very large in that state so that the uncertainty product remains greater than or equal to $\hbar/2$. In particular, if $\Delta x \to 0$, then $\Delta p_x \to \infty$ in such a manner that $\Delta x \Delta p_x \geq \hbar/2$.

Minimum Uncertainty Product.

From ~~Equations~~ (16) and (17) and the comments made after Eq. (22), the uncertainty product in Eq. (23) would be equal to the right hand side if the following two conditions are met:

$$(\hat{B} - \langle \hat{B} \rangle)|\psi\rangle = \lambda (\hat{A} - \langle \hat{A} \rangle)|\psi\rangle \quad \cdots\cdots (25)$$

where λ is a constant, and

$$\{\hat{A}', \hat{B}'\} = 0 \quad \cdots\cdots\cdots (26)$$

where $\hat{A}'$ and $\hat{B}'$ are defined as

$$\hat{A}' = \hat{A} - \langle \hat{A} \rangle$$
$$\hat{B}' = \hat{B} - \langle \hat{B} \rangle .$$

Now, from Eq. (25) we have

$$\langle \psi | (\hat{A} - \langle \hat{A} \rangle)(\hat{B} - \langle \hat{B} \rangle)|\psi\rangle = \lambda \langle \psi | (\hat{A} - \langle \hat{A} \rangle)^2 |\psi\rangle$$

or

$$\langle \psi | (\hat{A} - \langle \hat{A} \rangle)(\hat{B} - \langle \hat{B} \rangle)|\psi\rangle = \lambda (\Delta A)^2 . \quad \cdots\cdots (27)$$

From Eq. (25) we also have

$$\langle\psi|(\hat{B}-\langle\hat{B}\rangle)(\hat{A}-\langle\hat{A}\rangle)|\psi\rangle = \frac{1}{\lambda}(\Delta B)^2 \quad \cdots\cdots (28)$$

Adding Eqs. (27) and (28) and noting that

$$\hat{A}' \equiv \hat{A} - \langle\hat{A}\rangle$$
$$\hat{B}' \equiv \hat{B} - \langle\hat{B}\rangle$$

we have

$$\langle\psi|\{\hat{A}', \hat{B}'\}|\psi\rangle = \lambda(\Delta A)^2 + \frac{1}{\lambda}(\Delta B)^2 .$$

Since, one of the conditions for the uncertainty product to be minimum is that $\{\hat{A}', \hat{B}'\} = 0$ (Eq. (26)),

we have

$$\lambda(\Delta A)^2 + \frac{1}{\lambda}(\Delta B)^2 = 0 \quad \cdots\cdots\cdots (29)$$

Next, subtracting Eq. (28) from Eq. (27) we get

$$\langle\psi|(\hat{A}-\langle\hat{A}\rangle)(\hat{B}-\langle\hat{B}\rangle) - (\hat{B}-\langle\hat{B}\rangle)(\hat{A}-\langle\hat{A}\rangle)|\psi\rangle$$
$$= \lambda(\Delta A)^2 - \frac{1}{\lambda}(\Delta B)^2$$

or $$\langle\psi|[\hat{A},\hat{B}]|\psi\rangle = \lambda(\Delta A)^2 - \frac{1}{\lambda}(\Delta B)^2$$

or $$\langle[\hat{A},\hat{B}]\rangle = \lambda(\Delta A)^2 - \frac{1}{\lambda}(\Delta B)^2 \quad \cdots\cdots (30).$$

Finally adding Eqs. (29) and (30) we find

$$2\lambda(\Delta A)^2 = \langle[\hat{A},\hat{B}]\rangle$$

or
$$\lambda = \frac{\langle[\hat{A},\hat{B}]\rangle}{2(\Delta A)^2} \quad \cdots\cdots (31)$$

Substituting Eq. (31) in Eq. (25) we obtain the condition for the uncertainty product to be a minimum:

$$(\hat{B} - \langle\hat{B}\rangle)|\psi\rangle = \frac{\langle[\hat{A},\hat{B}]\rangle}{2(\Delta A)^2}(\hat{A} - \langle\hat{A}\rangle)|\psi\rangle. \quad \cdots (32)$$

If the state $|\psi\rangle$ of the system satisfies the above equation, the uncertainty product $\Delta A \Delta B$ would be minimum.

As an example, let
$$\hat{A} = \hat{x} = x, \text{ and } \hat{B} = \hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

Then, in coordinate representation, Eq (24) is

$$\left(\frac{\hbar}{i}\frac{\partial}{\partial x} - \langle p_x\rangle\right)\psi(x) = \frac{i\hbar}{2(\Delta x)^2}(x - \langle x\rangle)\psi(x)$$

i.e.,

$$\frac{d\psi(x)}{dx} = -\frac{(x-\langle x\rangle)}{2(\Delta x)^2}\psi(x) + \frac{i}{\hbar}\langle p_x\rangle\psi(x)$$

or $$\psi(x) = C\exp\left[\frac{-(x-\langle x\rangle)^2}{4(\Delta x)^2} + \frac{i}{\hbar}\langle p_x\rangle x\right]$$

where C is a constant. Normalising the wave function we have

$$\psi(x) = \frac{1}{\left[(2\pi)(\Delta x)^2\right]^{1/4}}\exp\left[-\frac{(x-\langle x\rangle)^2}{4(\Delta x)^2} + \frac{i}{\hbar}\langle p_x\rangle x\right] \quad \cdots (33)$$

If a particle, moving along the x-axis, has the wavefunction given by (26), with any value for $\langle x\rangle$ and $\langle p_x\rangle$, the uncertainty product $\Delta x \Delta p_x$ would have the minimum value given by

$$\Delta x\,\Delta p_x = \frac{\hbar}{2}.$$

Example.

The wave packet (i.e., wave function) for a free particle at $t = 0$, is given by

$$\psi(x) = N \exp\left[-\frac{(x - x_0)^2}{2\sigma^2} + i p_0 x/\hbar\right]$$

where N is a constant.

(a) Normalize the wave function.

(b) Find Δx, Δp and $\Delta x \cdot \Delta p$ at $t = 0$

Ans:

(a) $\langle \psi | \psi \rangle = 1$

i.e., $$\int_{-\infty}^{\infty} \psi^*(x)\, \psi(x)\, dx = 1$$

$$\propto \quad |N|^2 \int_{-\infty}^{\infty} e^{-(x - x_0)^2/\sigma^2}\, dx = 1 \qquad \Bigg| \quad \int_{-\infty}^{\infty} e^{-\alpha y^2}\, dy = \sqrt{\frac{\pi}{\alpha}}$$

$$\propto \quad |N|^{-2} \sqrt{\pi\sigma^2} = 1$$

$$\therefore \quad |N| = \frac{1}{(\pi\sigma^2)^{1/4}}$$

We choose N to be real and positive,

$$N = \frac{1}{(\pi\sigma^2)^{1/4}} .$$

$\therefore$ The normalized wave function is

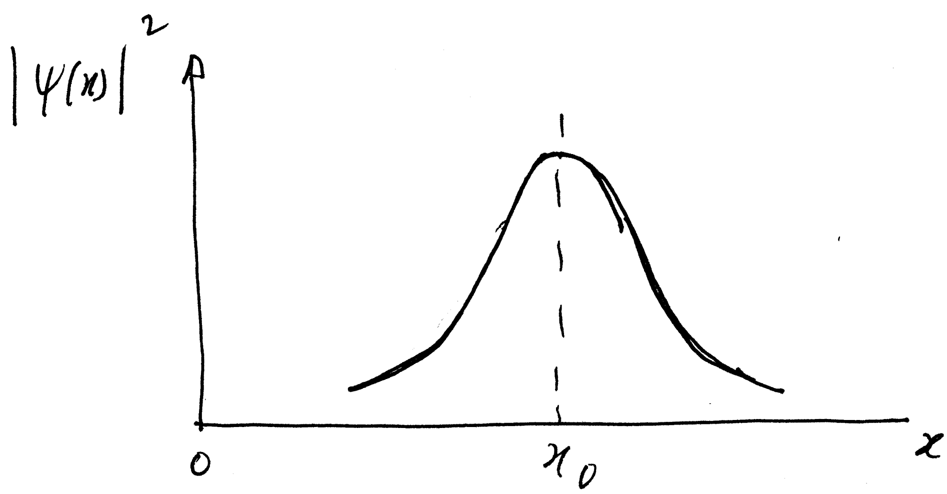
$$\psi(x) = \frac{1}{(\pi\sigma^2)^{1/4}} \exp\left[- \frac{(x-x_0)^2}{2\sigma^2} + i\, p_0 x/\hbar \right] .$$

(b) The normalized wave function is

$$\psi(x) = \frac{1}{(\pi\sigma^2)^{1/4}} \exp\left[- \frac{(x-x_0)^2}{2\sigma^2} + \frac{i}{\hbar} p_0 x \right]$$

$\therefore$ The position probability density is

$$|\psi(x)|^2 = \frac{1}{(\pi\sigma^2)^{1/2}} \exp\left[- \frac{(x-x_0)^2}{\sigma^2} \right]$$



The graph is symmetric around x_0.

$\therefore \ \langle x \rangle = x_0$.

Now we will calculate Δx.

$$(\Delta x)^2 = \langle (\hat{x} - \langle x \rangle)^2 \rangle$$

$$= \langle (\hat{x} - x_0)^2 \rangle$$

$$= \int_{-\infty}^{\infty} \psi^*(x)(x - x_0)^2 \psi(x)\, dx$$

$$= \frac{1}{(\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} (x - x_0)^2 e^{-(x-x_0)^2/\sigma^2} dx$$

$$= \frac{1}{(\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} u^2 e^{-u^2/\sigma^2} du \qquad \Big|\ u = x - x_0$$

$$= \frac{1}{(\pi\sigma^2)^{1/2}} \cdot \frac{\sigma^2}{2} (\pi\sigma^2)^{1/2} \qquad \Big|\ \int_{-\infty}^{\infty} u^2 e^{-\alpha u^2} = \frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}}$$

$$= \sigma^2/2$$

$$\therefore \boxed{\Delta x = \sigma/\sqrt{2}}$$

Now we will find $\langle p \rangle$ and Δp.

We can proceed in two ways. We can do the calculation in coordinate space (i.e., coordinate representation) and use $\hat{p} \to \frac{\hbar}{i}\frac{\partial}{\partial x}$. Alternatively, we can work in momentum space (momentum representation). We will then have to find the wavefunction in momentum representation $\tilde{\psi}(p)$ and use $\hat{p} \to p$ (multiplicative operator).

Let us work in coordinate representation. Finding $\langle p \rangle$ and Δp using momentum representation is given in the next example.

Let us first find $\langle p \rangle$.

$$\langle p \rangle = \langle \psi | \hat{p} | \psi \rangle$$

$$= \int_{-\infty}^{\infty} \psi^*(x) \, \frac{\hbar}{i} \frac{\partial}{\partial x} \psi(x) \, dx$$

$$= \frac{\hbar}{i} \cdot \frac{1}{(\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} e^{-(x-x_0)^2/2\sigma^2 - i p_0 x/\hbar} \frac{\partial}{\partial x} e^{-(x-x_0)^2/2\sigma^2 + i p_0 x/\hbar} \, dx$$

$$= \frac{\hbar}{i} \frac{1}{(\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} e^{-(x-x_0)^2/\sigma^2} \left[-\frac{(x-x_0)}{\sigma^2} + \frac{i p_0}{\hbar} \right] dx$$

$$= \frac{\hbar}{i} \frac{1}{(\pi\sigma^2)^{1/2}} \left[-\frac{1}{\sigma^2} \underbrace{\int_{-\infty}^{\infty} e^{-u^2/\sigma^2} u \, du}_{\substack{=0 \\ \text{integrand antisymmetric}}} + \frac{i p_0}{\hbar} \int_{-\infty}^{\infty} e^{-u^2/\sigma^2} du \right]$$

$$= \frac{\hbar}{i} \frac{1}{(\pi\cancel{\sigma^2})^{1/2}} \cdot \frac{i p_0}{\hbar} \cdot (\pi \cancel{\sigma^2})^{1/2} \qquad \Big| \; \int_{-\infty}^{\infty} e^{-\alpha u^2} du = \sqrt{\pi/\alpha}, \quad \alpha = \frac{1}{\sigma^2}$$

$$= p_0$$

Next, calculate Δp.

$$(\Delta p)^2 = \langle\psi|(\hat{p} - \langle\hat{p}\rangle)^2|\psi\rangle$$

$$= \langle\psi|\hat{p}^2|\psi\rangle - \langle\hat{p}\rangle^2$$

$$= \langle p^2\rangle - p_0^2 .$$

Now

$$\langle p^2\rangle = \langle\psi|\hat{p}^2|\psi\rangle . \quad \Big| \hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$= \frac{-\hbar^2}{(\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} e^{-(x-x_0)^2/2\sigma^2 - ip_0x/\hbar} \frac{\partial^2}{\partial x^2} e^{-(x-x_0)^2/2\sigma^2 + ip_0x/\hbar} dx$$

(integrate by parts)

$$= \frac{\hbar^2}{(\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} \left[\frac{\partial}{\partial x} e^{-(x-x_0)^2/2\sigma^2 - ip_0x/\hbar}\right]\left[\frac{\partial}{\partial x} e^{-(x-x_0)^2/2\sigma^2 + ip_0x/\hbar}\right] dx$$

$$= \frac{\hbar^2}{(\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} \underbrace{\left(-\frac{(x-x_0)}{\sigma^2} - i\frac{p_0}{\hbar}\right)\left(-\frac{(x-x_0)}{\sigma^2} + i\frac{p_0}{\hbar}\right)}_{\cancel{\text{cross term integrates to}}} e^{-(x-x_0)^2/\sigma^2} dx$$

$$= \frac{\hbar^2}{(\pi\sigma^2)^{1/2}} \left[\frac{1}{\sigma^4}\int_{-\infty}^{\infty}(x-x_0)^2 e^{-(x-x_0)^2/\sigma^2} + \frac{p_0^2}{\hbar^2}\int_{-\infty}^{\infty} e^{-(x-x_0)^2/\sigma^2} dx\right]$$

$$= \frac{\hbar^2}{\cancel{(\pi\sigma^2)^{1/2}}}\left[\frac{1}{\sigma^4}\cdot\frac{\sigma^2}{2}\cancel{(\pi\sigma^2)^{1/2}} + \frac{p_0^2}{\hbar^2}\cdot\cancel{(\pi\sigma^2)^{1/2}}\right]$$

$$= \frac{\hbar^2}{2\sigma^2} + p_0^2$$

$$\therefore (\Delta p)^2 = \frac{\hbar^2}{2\sigma^2} + p_0^2 - p_0^2 = \frac{\hbar^2}{2\sigma^2}$$

or $\quad \Delta p = \dfrac{\hbar}{\sqrt{2}\,\sigma}$.

Hence

$$\Delta x \,.\, \Delta p_x = \frac{\sigma}{\sqrt{2}} \cdot \frac{\hbar}{\sqrt{2}\,\sigma} = \frac{\hbar}{2}.$$

i.e., the uncertainty product is minimum.

Ex The normalized coordinate space wave function for a particle undergoing one-dimensional motion is given by

$$\psi(x) = \frac{1}{(\pi\sigma^2)^{1/4}} e^{-(x-x_0)^2/2\sigma^2 + i p_0 x/\hbar}$$

(a) Find the wave function in momentum space $\tilde{\psi}(p)$.

(b) From $\tilde{\psi}(p)$ find $\langle p \rangle$ and Δp.

Ans

(a) In momentum representation, the wave function of the particle is

$$\tilde{\psi}(p) \equiv \langle p|\psi\rangle = \int_{-\infty}^{\infty} \langle p|x\rangle\langle x|\psi\rangle \, dx$$

$$= \int_{-\infty}^{\infty} \langle p|x\rangle \, \psi(x) \, dx .$$

Now, the momentum eigenket $|p\rangle$ in the coordinate representation is

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}.$$

Therefore

$$\langle p|x\rangle = \langle x|p\rangle^* = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}.$$

Hence

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{(\pi\sigma^2)^{1/4}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} e^{-(x-x_0)^2/2\sigma^2 + ip_0x/\hbar} dx$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \cdot \frac{1}{(\pi\sigma^2)^{1/4}} \int_{-\infty}^{\infty} e^{-(x-x_0)^2/2\sigma^2 - i(p-p_0)x/\hbar} dx$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \cdot \frac{1}{(\pi\sigma^2)^{1/4}} \int_{-\infty}^{\infty} e^{-(x-x_0)^2/2\sigma^2 - i(p-p_0)(x-x_0)/\hbar} \cdot e^{-i(p-p_0)x/\hbar} dx$$

Letting $u = x - x_0$, we have

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \cdot \frac{1}{(\pi\sigma^2)^{1/4}} e^{-i(p-p_0)x/\hbar} \int_{-\infty}^{\infty} e^{-u^2/2\sigma^2 - i(p-p_0)u/\hbar} du$$

We now use the standard integral

$$\int_{-\infty}^{\infty} e^{-ax^2 - ikx}\, dx = \sqrt{\frac{\pi}{a}}\; e^{-k^2/4a} .$$

In our case

$$a = \frac{1}{2\sigma^2}, \quad \cancel{k = \ldots}$$

$$k = (p - p_0)/\hbar .$$

We find

$$\tilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \frac{1}{(\pi\sigma^2)^{1/4}} e^{-i(p-p_0)x_0/\hbar} \cdot \sqrt{2\pi\sigma^2} \cdot e^{-(p-p_0)^2/2(\hbar^2/\sigma^2)}$$

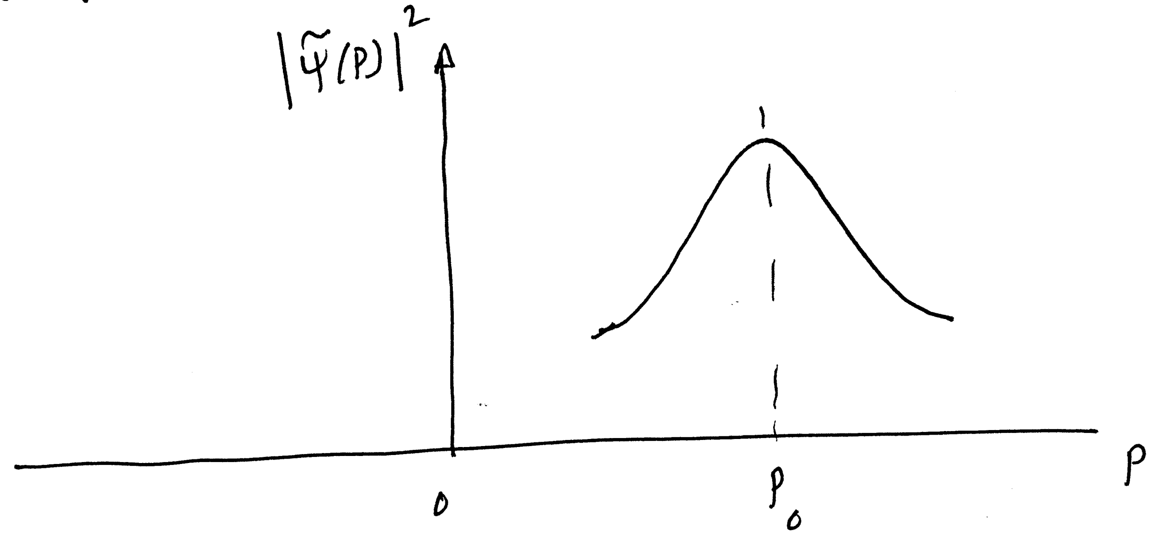
$$\boxed{\tilde{\psi}(p) = \frac{\sigma}{(\pi\hbar^2\sigma^2)^{1/4}} \exp\left[-\frac{(p-p_0)^2}{2(\hbar^2/\sigma^2)} - i(p-p_0)x_0/\hbar\right].}$$

(b) We have found the momentum space wave function $\tilde{\psi}(p)$ of the particle. Therefore, momentum probability density $\rho(p)$ is

$$\rho(p) \equiv \left|\tilde{\varphi}(p)\right|^2$$

$$= \frac{\sigma}{\sqrt{\pi}\,\hbar} \exp\left[- \frac{(p-p_0)^2}{(\hbar^2/\sigma^2)}\right]$$

The momentum probability density is peaked at $p = p_0$:



Also $|\tilde{\varphi}(p)|^2$ is symmetric around p_0. Thus

$$\boxed{\langle p \rangle = p_0}$$

Next, we will find Δp. We have

$$(\Delta p)^2 = \langle (\hat{p} - \langle \hat{p} \rangle)^2 \rangle$$

$$= \langle \psi | (\hat{p} - \langle \hat{p} \rangle)^2 | \psi \rangle$$

$$= \int_{-\infty}^{\infty} dp \, \langle \psi | p \rangle \langle p | (\hat{p} - p_0)^2 | \psi \rangle$$

$$= \int_{-\infty}^{\infty} dp \, (p - p_0)^2 \langle \psi | p \rangle \langle p | \psi \rangle$$

$$= \int_{-\infty}^{\infty} dp \, (p - p_0)^2 \, |\tilde{\psi}(p)|^2$$

$$= \frac{\sigma}{\pi^{1/2} \hbar} \int_{-\infty}^{\infty} (p - p_0)^2 \cancel{\frac{1}{4}} \exp\left[- \frac{(p - p_0)^2}{\hbar^2/\sigma^2} \right] dp$$

$$= \frac{\sigma}{\pi^{1/2} \hbar} \cdot \frac{\hbar^2}{2\sigma^2} \sqrt{\frac{\pi \hbar^2}{\cancel{2}\sigma^2}}$$

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} x^2 dx = \frac{1}{2\alpha} \sqrt{\frac{\pi}{\alpha}}$$

Take $\alpha = \frac{\sigma^2}{\hbar^2}$

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

$$\therefore \boxed{\Delta p = \frac{\hbar}{\sqrt{2}\,\sigma}}$$

$$\therefore \Delta x \, \Delta p = \frac{\sigma}{\sqrt{2}} \cdot \frac{\hbar}{\sqrt{2}\,\sigma} = \frac{\hbar}{2},$$

i.e., the uncertainty product is minimum.

Ex Lower bounds for ground state energy.

As we will see later, the variational principle can be used to find upper bounds of ground state energies. The uncertainty principle can be used to find lower bounds for the ground state energy of certain systems. We will use the uncertainty principle in the form $\Delta x \Delta p \geq \hbar/2$ to find rigorous lower bounds for the ground-state energy of one-dimensional Hamiltonians. This is best illustrated by an example.

Ex 1 Consider a particle in a one-dimensional quartic potential

$$V(\hat{x}) = \alpha \hat{x}^4 \quad \ldots \quad (1)$$

where $\alpha > 0$ is a constant with units of energy over length to the fourth power. Our goal is to find a lower bound for the ground state energy $\langle H \rangle_{gs}$.

The Hamiltonian operator for the particle is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \alpha \hat{x}^4 , \quad \cdots\cdots (2)$$

Therefore, taking the ground state expectation value we have

$$\langle \hat{H} \rangle_{gs} = \frac{\langle \hat{p}^2 \rangle_{gs}}{2m} + \alpha \langle \hat{x}^4 \rangle_{gs} . \quad \cdots\cdots (3)$$

Now, recalling that

$$(\Delta p)^2 = \langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2$$

i.e., $\langle \hat{p}^2 \rangle = (\Delta p)^2 + \langle \hat{p} \rangle^2$

we see that

$$\langle \hat{p}^2 \rangle \geq \quad \cdots\cdots (4)$$

the equality holds if $\langle \hat{p} \rangle = 0$. Eq. (4) is true for any state. Now, for a bound state in a symmetric potential, $\langle \hat{p} \rangle = 0$. Therefore we actually have

$$\langle \hat{p}^2 \rangle_{gs} = (\Delta p)^2_{gs} \quad \cdots\cdots (5)$$

Expectation value of $\hat{x}^4$.

Recall that for any operator $\hat{A}$,

$$(\Delta A)^2 = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2$$

i.e., $$\langle \hat{A}^2 \rangle = (\Delta A)^2 + \langle \hat{A} \rangle^2.$$

From this we have two inequalities

$$\langle \hat{A}^2 \rangle \geq \langle \hat{A} \rangle^2 \quad (\text{Equality holds if } \Delta A = 0)$$

and $$\langle \hat{A}^2 \rangle \geq (\Delta A)^2 \quad (\text{Equality holds if } \langle \hat{A} \rangle = 0).$$

Now, from the inequality $\langle \hat{A}^2 \rangle \geq \langle \hat{A} \rangle^2$, we have

$$\langle \hat{x}^4 \rangle \geq \langle \hat{x}^2 \rangle^2$$

From the inequality $\langle \hat{A}^2 \rangle \geq (\Delta A)^2$ we have

$$\langle \hat{x}^2 \rangle \geq (\Delta x)^2$$

so that $$\boxed{\langle \hat{x}^4 \rangle \geq (\Delta x)^4.} \quad \text{-------}$$

Equation (6) is valid for any state, so, in particular it is valid for the ground state also.

Therefore,

$$\langle H \rangle_{gs} = \frac{\langle \hat{p}^2 \rangle_{gs}}{2m} + \alpha \langle \hat{x}^4 \rangle_g$$

$$\geqslant \frac{(\Delta p_{gs})^2}{2m} + \alpha \, (\Delta x_{gs})^4 . \quad \cdots\cdots (7)$$

From the uncertainty principle,

$$\Delta x_{gs} \, \Delta p_{gs} \geqslant \frac{\hbar}{2} \longrightarrow \Delta p_{gs} \geqslant \frac{\hbar}{2 \Delta x_{gs}} .$$

Back to $\langle H \rangle_{gs}$ we get

$$\langle H \rangle_{gs} \geqslant \frac{\hbar^2}{8m (\Delta x_{gs})^2} + \alpha (\Delta x_{gs})^4 . \quad \cdots (8)$$

The quantity on the right hand side is a function of Δx_{gs}. This function is plotted in the figure below:

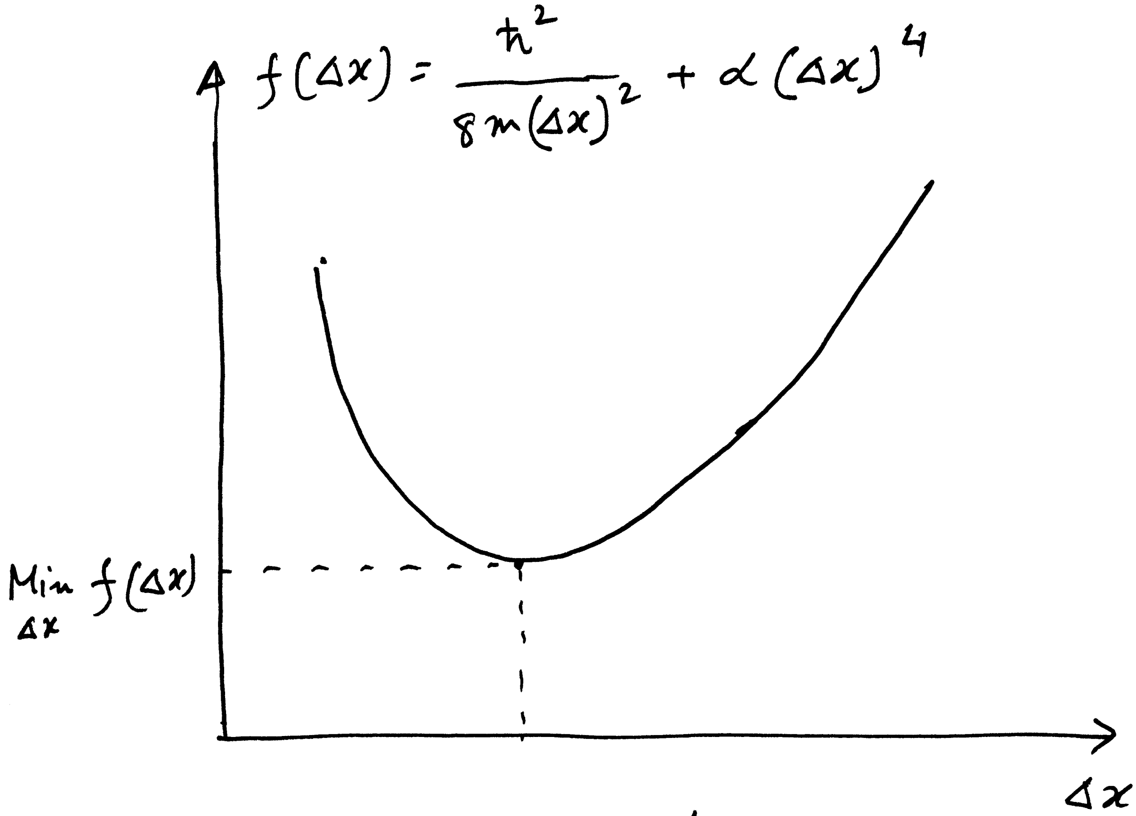


Figure: We have that $\langle \hat{H} \rangle_{gs} \geq f(\Delta x_{gs})$, But we don't know the value of Δx_{gs}. As a result, we can only be certain that $\langle H \rangle_{gs}$ is greater than or equal to the lowest value the function $f(\Delta x_{gs})$ can take.

If we knew the value of Δx_{gs}, we would immediately know that $\langle H \rangle_{gs}$ is bigger than the value taken by the right side of Eq. (8). This would be quite nice, since we want the highest possible lower bound. Since we don't know the value of Δx_{gs}, the only thing we can be sure of is that $\langle H \rangle_{gs}$ is bigger than the lowest value that the right hand side of Eq. (8) can take as we vary Δx_{gs}. Thus

$$\langle H \rangle_{gs} \geq \operatorname*{Min}_{\Delta x} \left(\frac{\hbar^2}{8m(\Delta x)^2} + \alpha (\Delta x)^4 \right). \quad \cdots (9)$$

The minimization problem is straightforward. In fact a function $f(u)$ given by

$$f(u) = \frac{\hbar^2}{8mu^2} + \alpha u^4$$

is minimized for

$$u^2 = \left(\frac{\hbar^2}{16 m \alpha} \right)^{1/3}$$

Hence

$$\langle H \rangle_{gs} \geq \frac{\hbar^2}{8m \left(\frac{\hbar^2}{16 m\alpha} \right)^{1/3}} + \alpha \left(\frac{\hbar^2}{16 m\alpha} \right)^{2/3}.$$

Simplifying, we get

$$\langle H \rangle_{gs} \geq 2^{1/3} \frac{3}{8} \left(\frac{\hbar^2 \sqrt{\alpha}}{m} \right)^{2/3} \cong 0.4724 \left(\frac{\hbar^2 \sqrt{\alpha}}{m} \right)^{2/3}.$$

This is the final lower bound for the ground state energy. It is actually not too bad, for the exact ground state energy, the prefactor is 0.668 instead of 0.4724.