UNIVERSITÀ DEGLI STUDI DI MILANO BICOCCA

Position and momentum operators, uncertainty principle

Hermitian Operators and Observables

1. "Every observable is represented in quantum theory by a Hermitian operator"

2. "If an operator is created to represent an observable,
its eigenvalues indicate possible values of a measurement of that observable,
and the eigenstates define the quantum state of the system"

So far, the only operator we have considered has been the Hamiltonian $\hat{H}$ associated with the energy E.

We can construct operators associated with many other measurable quantities.

Momentum and momentum operator

We may consider the momentum operator corresponding to the classical momentum **p**: $\mathbf{p} \rightarrow \hat{\boldsymbol{p}}$

$|p\rangle$ here are eigenvectors of $\hat{\boldsymbol{p}}$ and so $\hat{\boldsymbol{p}}\ |p\rangle = \lambda_p\ |p\rangle$

We postulate that:

$$\hat{\boldsymbol{p}} \equiv -i\hbar\nabla$$

Momentum and momentum operator

We postulate that:

$$\hat{\boldsymbol{p}} \equiv -i\hbar\nabla$$

Thus:

$$\frac{\hat{\boldsymbol{p}}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2$$

Linking the classical notion of the energy E

$$E = \frac{\boldsymbol{p}^2}{2m} + V$$

To the Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V = \frac{\hat{\boldsymbol{p}}^2}{2m} + \hat{V}$$

Momentum and momentum operator

$$\hat{\boldsymbol{p}} \equiv -i\hbar\nabla$$

The plane wave $e^{i\mathbf{K}\cdot\mathbf{r}}$ are solutions of the eigenvector equation for the $\hat{\boldsymbol{p}}$ operator, in fact:

$$\hat{\boldsymbol{p}}\ e^{i\mathbf{K}\cdot\mathbf{r}} = \hbar\mathbf{K}\ e^{i\mathbf{K}\cdot\mathbf{r}}$$

with $\hbar\mathbf{K}$ being the corresponding eigenvalues

Thus, we can also write that the momentum **p** is:

$$\mathbf{p} = \hbar\mathbf{K}$$

This $\mathbf{p}$ represents possible values of measurements of the momentum of the system, and note that it is in general a vector.

Position and position operator

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The corresponding operator is almost trivial when we are working with functions of position .

It is simply the position vector, r, itself.

We typically do not write $\hat{r}$, though rigorously we should.

Uncertainty principle

We cannot simultaneously know both the position and momentum of a particle.

We have already seen, for the example of a gaussian wave packet, that:

$$\Delta x \, \Delta k = \frac{1}{2}$$

Or, considering the momentum $\mathbf{p} = \hbar \mathbf{K}$

$$\Delta x \, \Delta p = \frac{\hbar}{2}$$

Uncertainty principle

The Gaussian distribution and its Fourier transform have the minimum product $\Delta k \Delta x$ of any distribution

Thus, we can state the uncertainty principle as:

$$\Delta x \, \Delta p \geq \frac{\hbar}{2}$$

Though demonstrated here only for a specific example, this uncertainty principle is quite general (for all observables not mutually-exclusive, e.g. freq. and time)

Uncertainty principle

The Gaussian distribution and its Fourier transform have the minimum product ΔkΔx of any distribution

Thus, we can state the uncertainty principle as:

$$\Delta x\, \Delta p \geq \frac{\hbar}{2}$$

It is not merely that we cannot simultaneously measure these two quantities, but a particle simply does not have simultaneously both a well-defined position and a well-defined momentum.

Expectation value

$$\langle \alpha | \hat{T} | \alpha \rangle = \langle T \rangle = \sum_n \sum_m a_n^* a_m \langle \chi_n | \hat{T} | \chi_m \rangle$$

$\hat{T}|\chi_m\rangle = \lambda_m \chi_m$

$$= \sum_n \sum_m a_n^* a_m \lambda_m \langle \chi_n | \chi_m \rangle$$

δ_{nm}

$$= \sum_n |a_n|^2 \lambda_n$$

probability of getting λ_n

It has the meaning of the average value of the observable, which one would "expect" to find if the same measurement is repeated multiple times

Standard deviation

The results of the different measurements of $\hat{T}$ will be scattered around the expectation value, $\langle \hat{T} \rangle$. The statistical uncertainty of such measurements is the standard deviation

$$\sigma_T \equiv \sqrt{\langle \hat{T}^2 \rangle - \langle T \rangle^2}$$

in general for discrete observ.

$$\sigma_x \equiv \sqrt{\langle \hat{x}^2 \rangle - \langle x \rangle^2} = \sqrt{\int_{-\infty}^{\infty} (x - \langle x \rangle)^2 \, |\psi|^2 \, dx}$$

for the x contin. observ.

σ_x^2 is the variance of x

Standard deviation

$$\sigma_x \equiv \sqrt{\langle \hat{x}^2 \rangle - \langle x \rangle^2} = \sqrt{\int_{-\infty}^{\infty} (x - \langle x \rangle)^2 \ |\psi|^2 \, dx} = \sqrt{\langle (\hat{x} - \langle x \rangle)^2 \rangle}$$

σ_x^2 is the variance of x

$$\Delta x = x - \langle x \rangle$$

deviation from mean value

$$\langle \Delta x \rangle = 0$$

average of scattering is zero

$$\langle (\Delta x)^2 \rangle = \left\langle (x - \langle x \rangle)^2 \right\rangle = \left\langle x^2 - 2x\langle x \rangle + \langle x \rangle^2 \right\rangle$$

$$= \langle x^2 \rangle - 2\langle x \rangle \langle x \rangle + \langle x \rangle^2 = \langle x^2 \rangle - \langle x \rangle^2$$

Standard deviation

$$\sigma_x \equiv \langle (\hat{x} - \langle x \rangle)^2 \rangle$$

if $\sigma_x = 0$ => $(\hat{x} - \langle x \rangle) = 0$

That means that:

$$\hat{x}\psi = \langle x \rangle \psi$$

Thus:

If $\langle x \rangle$ coincides with an eigenvalue of the operator, then the uncertainty in the measurement is zero.

This is what we have already discussed: if the state of the system is an eigenstate, then the corresponding eigenvalue coincides with the expectation value of the measurement and the standard deviation is zero.

Generalized Uncertainty Principle

Let us define an operator associated with the variance of A

$$\sigma_A^2 \equiv \langle \hat{A}^2 \rangle - \langle A \rangle^2 = \left\langle \left(\hat{A} - \langle A \rangle \right)^2 \right\rangle =$$

Thus, $\sigma_A^2 = \left\langle \psi \middle| \left(\hat{A} - \langle A \rangle \right)^2 \middle| \psi \right\rangle = \left\langle \psi \middle| \left(\hat{A} - \langle A \rangle \right)^\dagger \left(\hat{A} - \langle A \rangle \right) \middle| \psi \right\rangle =$

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

Similarly, for $\hat{B}$

$$\sigma_B^2 = \langle g | g \rangle$$

Generalized Uncertainty Principle

Thus

$$\sigma_A^2 \sigma_B^2 = \langle f|f\rangle\langle g|g\rangle \geq |\langle f|g\rangle|^2$$

Because of Schwartz inequality stating

$$\left|\int_a^b f^*(x)\, g(x)\, dx\right|^2 \leq \int_a^b |f(x)|^2\, dx \int_a^b |g(x)|^2\, dx$$

If z is a complex number $z = \langle f|g\rangle$:

$$|z|^2 = [\mathrm{Re}(z)]^2 + [\mathrm{Im}(z)]^2 \geq [\mathrm{Im}(z)]^2 = \left[\frac{1}{2\,i}\,(z - z^*)\right]^2$$

Generalized Uncertainty Principle

Thus

$$\sigma_A^2\,\sigma_B^2 \geq \left[\frac{1}{2\,i}\,(z - z^*)\right]^2$$

One can show that

$\langle f|g\rangle$=z= $\langle \hat{A}\hat{B}\rangle - \langle A\rangle\langle B\rangle$

$\langle g|f\rangle$=z*= $\langle \hat{B}\hat{A}\rangle - \langle A\rangle\langle B\rangle$

Thus

z-z*= $\langle \hat{A}\hat{B}\rangle - \langle \hat{B}\hat{A}\rangle = \langle[\hat{A},\hat{B}]\rangle$

Finally:

$$\sigma_A^2\,\sigma_B^2 \geq \left[\frac{1}{2i}\,\langle[\hat{A},\hat{B}]\rangle\right]^2$$

Generalized Uncertainty Principle

Let's consider the canonical commutation relation:

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

In fact:

$$\hat{\boldsymbol{p}} \equiv -i\hbar \frac{d}{dx}$$

and

$$\hat{\boldsymbol{p}}|f\rangle = -i\hbar \frac{d}{dx}|f\rangle$$

Thus:

$$[\hat{\boldsymbol{p}}, \boldsymbol{x}]|f\rangle = -i\hbar\left(\frac{d}{dx}x - x\frac{d}{dx}\right)|f\rangle =$$

$$-i\hbar\left[\frac{d}{dx}(x|f\rangle) - x\frac{d}{dx}|f\rangle\right] = -i\hbar\left[\left(\frac{d}{dx}x\right)|f\rangle + x\frac{d}{dx}|f\rangle - x\frac{d}{dx}|f\rangle\right] = -i\hbar|f\rangle$$

Generalized Uncertainty Principle

$$\sigma_A^2 \, \sigma_B^2 \geq \left[\frac{1}{2\,i} \langle [\hat{A}, \hat{B}] \rangle \right]^2$$

If we consider the canonical commutation relation:

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

Then

$$\sigma_x^2 \, \sigma_p^2 \geq \left[\frac{1}{2\,i} \, i\hbar \right]^2 = \left(\frac{\hbar}{2}\right)^2$$

This is the original Heisenberg uncertainty principle

$$\Delta x \, \Delta p \geq \frac{\hbar}{2}$$

Time evolution operator

S.E. $i\hbar \frac{d|\alpha\rangle}{dt} = \hat{H}|\alpha\rangle$ or $\frac{d}{dt}|\alpha\rangle = -\frac{i}{\hbar}\hat{H}|\alpha\rangle$

If the Hamiltonian $\hat{H}$ is constant in time a very simple solution can be obtained by integrating this:

$$|\alpha(t)\rangle = \exp(-i\frac{\hat{H}}{\hbar}t)\ |\alpha_0\rangle$$

where $|\alpha_0\rangle$ is the state of the system at time t=0

If it is legal to do that, we can have an operator that gives us the state at any time when applied to (or starting from) that at time t=0.

Time evolution operator

S.E. $$i\hbar \frac{d|\alpha\rangle}{dt} = \hat{H}|\alpha\rangle \quad \text{or} \quad \frac{d}{dt}|\alpha\rangle = -\frac{i}{\hbar}\hat{H}|\alpha\rangle$$

If the Hamiltonian $\hat{H}$ is constant in time a very simple solution is:

$$|\alpha(t)\rangle = \exp\left(-i\frac{\hat{H}}{\hbar}t\right)|\alpha_0\rangle$$

For practical calculations, the action of the exponent of an operator on a vector is not easy to compute…

Now, if we consider $|\alpha_0\rangle = |\chi_n\rangle$ to be an eigenvectors of $\hat{H}$ with eigenvalue E_n, then:

$$\hat{H}|\chi_n\rangle = E_n|\chi_n\rangle$$

Time evolution operator

S.E. $i\hbar \frac{d|\alpha\rangle}{dt} = \hat{H}|\alpha\rangle$ or $\frac{d}{dt}|\alpha\rangle = -\frac{i}{\hbar}\hat{H}|\alpha\rangle$

If the Hamiltonian $\hat{H}$ is constant in time a very simple solution is:

$$|\alpha(t)\rangle = \exp(-i\frac{\hat{H}}{\hbar}t)\,|\alpha_0\rangle$$

Operator of exponential function:

$$\exp(\hat{T}) = \sum_n \frac{1}{n!}\hat{T}^n$$

N.B. Power series of exponential functions

$$e^x = \sum_n \frac{x^n}{n!}$$

Time evolution operator

S.E. $i\hbar\frac{d|\alpha\rangle}{dt} = \hat{H}|\alpha\rangle$ or $\frac{d}{dt}|\alpha\rangle = -\frac{i}{\hbar}\hat{H}|\alpha\rangle$

If the Hamiltonian $\hat{H}$ is constant in time a very simple solution is:

$$|\alpha(t)\rangle = \exp(-i\frac{\hat{H}}{\hbar}t)\,|\alpha_0\rangle$$

$$\exp(\hat{T}) = \sum_n \frac{1}{n!}\hat{T}^n$$

Thus:

$$|\alpha(t)\rangle = \sum_m \frac{1}{m!}\left(\frac{-it}{\hbar}\right)^m \hat{H}^m|\alpha_0\rangle$$

Time evolution operator

$$|\alpha(t)\rangle = \exp(-i\frac{\hat{H}}{\hbar}t)\,|\alpha_0\rangle$$

Now, if we consider $|\alpha_0\rangle = |\chi_n\rangle$ to be an eigenvectors of $\hat{H}$ with eigenvalue E_n

$$|\alpha(t)\rangle = \sum_m \frac{1}{m!}\left(\frac{-\mathrm{i}t}{\hbar}\right)^m \hat{H}^m|\chi_n\rangle$$

Time evolution operator

$$|\alpha(t)\rangle = \exp(-i\frac{\hat{H}}{\hbar}t)\,|\alpha_0\rangle$$

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$$|\alpha(t)\rangle = \sum_m \frac{1}{m!}\left(\frac{-\mathrm{i}t}{\hbar}\right)^m \underbrace{\hat{H}^m|\chi_n\rangle}_{=\,E_n^m\,|\chi_n\rangle}$$

Time evolution operator

$$|\alpha(t)\rangle = \exp(-i\frac{\hat{H}}{\hbar}t)\,|\alpha_0\rangle$$

Now, if we consider $|\alpha_0\rangle = |\chi_n\rangle$ to be an eigenvectors of $\hat{H}$ with eigenvalue E_n

$$\hat{H}|\chi_n\rangle = E_n|\chi_n\rangle$$

$$|\alpha(t)\rangle = \sum_m \frac{1}{m!}\left(\frac{-\mathrm{i}t}{\hbar}\right)^m E_n^m|\chi_n\rangle = \exp(-i\frac{E_n}{\hbar}t)|\chi_n\rangle$$

Rewritten as exponential

Time evolution operator

$$|\alpha(t)\rangle = \exp(-i\frac{E_n}{\hbar}t)|\chi_n\rangle$$

This is the solution to the time-dependent Schrödinger equation, that we have also written as:

$$\psi(r,t) = \psi_n(r)\, e^{-i E_n t/\hbar}$$

Thus, if a system is initially in a state represented by an eigenstate, it remains in this state for ever: the time -dependent factor is a complex number and does not affect any measurable quantity, because its modulus squared is equal to unity

Time evolution operator

This is the solution to the time-dependent Schrödinger equation, that we have also written as:

$$\psi(r,t) = \psi_n(r)\, \mathrm{e}^{-\mathrm{i}\, E_n\, t/\hbar}$$

And we also now that a superposition state will be:

$$\Psi(x) = \sum_n c_n\, \psi_n(x)$$

And thus:

$$\Psi(r,t) = \sum_n c_n\, \psi_n(r)\, \mathrm{e}^{-\mathrm{i}\, E_n\, t/\hbar}$$

Time evolution operator

Starting with:

$$\Psi(r,t) = \sum_n c_n \, \psi_n(r) \, \mathrm{e}^{-\mathrm{i} E_n t/\hbar}$$

And by exploiting $\mathrm{e}^x = \sum_n \frac{x^n}{n!}$

$$\Psi(r,t) = \sum_n c_n \, \psi_n(r) \, \frac{(-\mathrm{i} E_n t/\hbar)^n}{\mathrm{n!}} = \sum_n c_n \, \frac{(-\mathrm{i}\, t/\hbar)^n}{n!} (E_n)^n \psi_n(r)$$

everywhere in the summation term we have $E_n \psi_n(r)$, we can substitute $\hat{H}\psi_n(r)$

Time evolution operator

$$\Psi(r,t) = \sum_n c_n\ \psi_n(r)\ \frac{(-\mathrm{i}\,E_n\,t/\hbar)^n}{\mathrm{n}!}$$

everywhere in the summation term we have $E_i\,\psi_i(r)$, we can substitute $\hat{H}\psi_i(r)$

$$\Psi(r,t) = \sum_n c_n\ \frac{(-\mathrm{i}\,\hat{H}t/\hbar)^n}{\mathrm{n}!}\psi_n(r)$$

And using $\Psi(x) = \sum_n c_n\ \psi_n(x)$

$$\Psi(r,t) = \Psi(r)\sum_n \frac{(-\mathrm{i}\,\hat{H}t/\hbar)^n}{n!}$$

Time evolution operator

$$\psi(r,t) = \psi(x)\sum_{n}\frac{(-i\hat{H}t/\hbar)^n}{n!}$$

And by exploiting again $e^x = \sum_n \frac{x^n}{n!}$

$$\Psi(r,t) = \Psi(r,t_0)e^{-i\hat{H}t/\hbar}$$

Hence, we have established that there is a well-defined operator that given the quantum mechanical wavefunction or "state" at time t=0 , will tell us what the state is at a time t.