

Position and momentum operators, uncertainty principle

Fundamentals of Quantum Mechanics for Materials Scientists

Hermitian Operators and Observables



- 1. "Every observable is represented in quantum theory by a Hermitian operator"
- 2. <u>"If an operator is created to represent an observable,</u> <u>its eigenvalues indicate possible values of a measurement of that observable,</u> <u>and the eigenstates define the quantum state of the system"</u>

- So far, the only operator we have considered has been the Hamiltonian \widehat{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**: $\mathbf{p} \rightarrow \hat{p}$

|p
angle here are eigenvectors of \widehat{p} and so

 $\widehat{\boldsymbol{p}} |p\rangle = \lambda_p |p\rangle$

We postulate that:

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

Momentum and momentum operator

We postulate that:

$$\widehat{\boldsymbol{p}} \equiv -i\hbar
abla$$

Thus:

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

Linking the classical notion of the energy E $E = \frac{p^2}{2m} + V$

To the Hamiltonian operator

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



Momentum and momentum operator



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

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

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

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



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:

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

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 $\Delta k \Delta x$ of any distribution

Thus, we can state the uncertainty principle as:

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

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 welldefined momentum.



Expectation value

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

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

$$\sigma_{x}^{2} \text{ is the variance of } x \qquad \Delta x = x - \langle x \rangle \qquad \text{oleventian} \text{ from mion volut}$$

$$\langle \Delta x \rangle = 0 \qquad \text{oleventian} \text{ of } x \text{ oleventian} \text{ oleventian} \text{ of } x \text{ oleventian} \text{ oleventian} \text{ oleventian} \text{ of } x \text{ oleventian} \text{ ol$$

Standard deviation



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

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

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.



Let us define an operator associated with the variance of A $\sigma_A^2 \equiv \langle \hat{A}^2 \rangle - \langle A \rangle^2 = \langle (\hat{A} - \langle A \rangle)^2 \rangle =$

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

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

Similarly, for \hat{B} $\sigma_B^2 = \langle g | g \rangle$



Thus

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

Because of Schwartz inequality stating $\left| \int_{a}^{b} f^{*}(x) g(x) dx \right|^{2} \leq \int_{a}^{b} |f(x)|^{2} dx \int_{a}^{b} |g(x)|^{2} dx$

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If z is a complex number z = \langle f | g \rangle:
|z|^2 = [\operatorname{Re}(z)]^2 + [\operatorname{Im}(z)]^2 \ge [\operatorname{Im}(z)]^2 = \left[\frac{1}{2i}(z-z^*)\right]^2
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Thus

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

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:

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



Let's consider the canonical commutation relation:

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

in fact:
$$\widehat{p} \equiv -i\hbar rac{d}{dx}$$

and
$$\widehat{p}|f
angle=-i\hbarrac{d}{dx}|f
angle$$

Thus:

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

Generalized Uncertainty Principle





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

If we consider the canonical commutation relation: $[\hat{x}, \hat{p}_x] = i\hbar$

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

This is the original Heisenberg uncertainty principle $\Delta x \, \Delta p \geq \frac{\hbar}{2}$



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

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

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

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.



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$$i\hbar \frac{d|\alpha\rangle}{dt} = \widehat{H}|\alpha\rangle$$
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If the Hamiltonian \widehat{H} is constant in time a very simple solution is:

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

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 \widehat{H} with eigenvalue E_n , then:

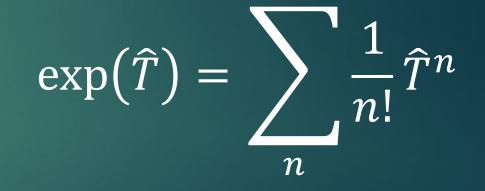
$$\widehat{H}|\chi_n\rangle = E_n|\chi_n\rangle$$



S.E.
$$i\hbar \frac{d|\alpha\rangle}{dt} = \widehat{H}|\alpha\rangle$$
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If the Hamiltonian \widehat{H} is constant in time a very simple solution is:

 $|\alpha(t)\rangle = \exp(-i\frac{\widehat{H}}{\hbar}t) |\alpha_0\rangle$ Operator of exponential function:



N.B. Power series of exponential functions

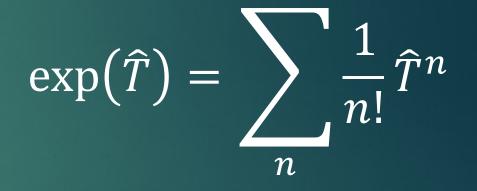
$$e^{x} = \sum_{n} \frac{x^{n}}{n!}$$



S.E.
$$i\hbar \frac{d|\alpha\rangle}{dt} = \widehat{H}|\alpha\rangle$$
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If the Hamiltonian \widehat{H} is constant in time a very simple solution is:

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



Thus:

$$|\alpha(t)\rangle = \sum_{m} \frac{1}{m!} \left(\frac{-it}{\hbar}\right)^{m} \widehat{H}^{m} |\alpha_{0}\rangle$$



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

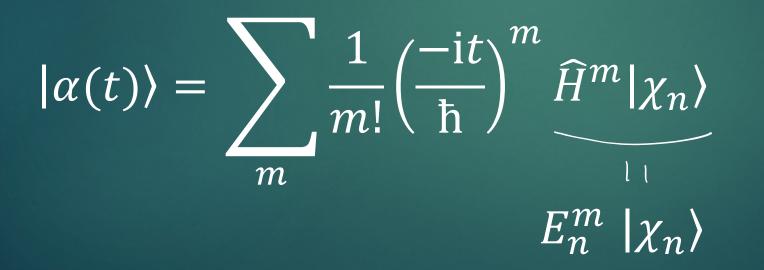
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$$|\alpha(t)\rangle = \sum_{m} \frac{1}{m!} \left(\frac{-it}{\hbar}\right)^{m} \widehat{H}^{m} |\chi_{n}\rangle$$



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

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

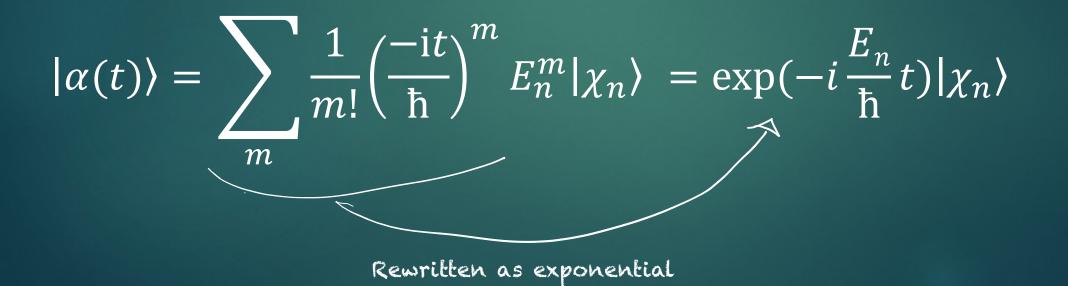




$$|\alpha(t)\rangle = \exp(-i\frac{\widehat{H}}{\hbar}t) |\alpha_0\rangle$$

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

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





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

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

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

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



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

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

And we also now that a superposition state will be: $\Psi(x) = \sum_{n} c_n \ \psi_n(x)$

And thus:

$$\Psi(r,t) = \sum_{n} c_n \psi_n(r) e^{-iE_n t/\hbar}$$



Starting with:

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

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

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

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



$$\Psi(r,t) = \sum_{n} c_n \psi_n(r) \frac{(-iE_n t/\hbar)^n}{n!}$$

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

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

And using $\Psi(x) = \sum_{n} c_{n} \psi_{n}(x)$

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



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

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.