4.3 Measurement and expectation values

Slides: Video 4.3.1 Quantum-mechanical measurement

Text reference: Quantum Mechanics for Scientists and Engineers

Section 3.8
Suppose we take some (normalized) quantum mechanical wave function $\Psi(r, t)$ and expand it in some complete orthonormal set of spatial functions $\psi_n(r)$.

At least if we allow the expansion coefficients $c_n$ to vary in time, we know we can always do this:

$$\Psi(r, t) = \sum_n c_n(t)\psi_n(r)$$
Probabilities and expansion coefficients

Then the fact that $\Psi(r,t)$ is normalized means we know the answer for the normalization integral

$$
\int_{-\infty}^{\infty} \left| \Psi(r,t) \right|^2 d^3r = \int_{-\infty}^{\infty} \left[ \sum_n c_n^*(t) \psi_n^*(r) \right] \times \left[ \sum_m c_m(t) \psi_m(r) \right] d^3r = 1
$$

Because of the orthogonality of the basis functions only terms with $n = m$ survive the integration. Because of the orthonormality of the basis functions the result from any such term will simply be $\left| c_n(t) \right|^2$

Hence we have $\sum_n |c_n|^2 = 1$
Measurement postulate

On measurement of a state
the system collapses into the $n$th eigenstate of the quantity being measured
with probability $P_n = |c_n|^2$

In the expansion of the state
in the eigenfunctions
of the quantity being measured
$c_n$ is the expansion coefficient
of the $n$th eigenfunction
Expectation value of the energy

Suppose do an experiment to measure the energy $E$ of some quantum mechanical system

We could repeat the experiment many times and get a statistical distribution of results.

Given the probabilities $P_n$ of getting a specific energy eigenstate, with energy $E_n$

we would get an average answer

$$\langle E \rangle = \sum_n E_n P_n = \sum_n E_n |c_n|^2$$

where we call this average $\langle E \rangle$ the "expectation value"
Energy expectation value example

For example, for the coherent state discussed above with parameter $N$, we have

$$
\langle E \rangle = \sum_{n=0}^{\infty} E_n \frac{N^n \exp(-N)}{n!} = \hbar \omega \left[ \sum_{n=0}^{\infty} n \frac{N^n \exp(-N)}{n!} \right] + \frac{1}{2} \hbar \omega = \left( N + \frac{1}{2} \right) \hbar \omega
$$

where we use the result that the average in a Poisson statistical distribution is just the parameter $N$.

Note that $N$ does not have to be an integer.

This is an expectation value, not an eigenvalue.

We can have states with any expectation value we want.
This apparatus has a non-uniform magnetic field locally stronger near the North pole magnet face because it is narrower.
Imagine firing some small magnets initially along the dashed line. Because the magnetic field is non-uniform, stronger near the North pole than near the South pole, a vertical magnet will be deflected up.
Stern-Gerlach experiment

Imagine firing some small magnets initially along the dashed line. Because the magnetic field is non-uniform, stronger near the North pole than near the South pole, a vertical magnet will be deflected up or down.
Stern-Gerlach experiment

A horizontally-oriented magnet will not be deflected
Stern-Gerlach experiment

A horizontally-oriented magnet will not be deflected and magnets of other orientations should be deflected by intermediate amounts. After “firing” many randomly oriented magnets we should end up with a line on the screen.
Electrons and the Stern-Gerlach experiment

Electrons have a quantum mechanical property called spin.

It gives them a “magnetic moment” just like a small magnet.

What will happen if we fire electrons with no particular “orientation” of their spin into the Stern-Gerlach apparatus?

We might expect the “line” on the screen.

(Note: the actual experiment used silver atoms, which behave the same as electrons in this case)
Stern-Gerlach experiment

With electrons we get two dots!

“Explanation”

We are measuring the vertical component of the spin.

There are two eigenstates of this component up and down so we have collapse to the eigenstates.
4.3 Measurement and expectation values

Slides: Video 4.3.3 Expectation values and operators

Text reference: Quantum Mechanics for Scientists and Engineers

Sections 3.9 – 3.10
Measurement and expectation values

Expectation values and operators

Quantum mechanics for scientists and engineers

David Miller
In classical mechanics, the Hamiltonian is a function of position and momentum representing the total energy of the system. In quantum mechanical systems that can be analyzed by Schrödinger’s equation we can define the entity
\[ \hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(r,t) \]
so we can write the Schrödinger equations as
\[ \hat{H}\psi(r) = E\psi(r) \quad \text{and} \quad \hat{H}\Psi(r,t) = i\hbar \frac{\partial \Psi(r,t)}{\partial t} \]
Hamiltonian operator

The entity $\hat{H}$

is not a number

is not a function

It is an “operator”

just like the entity $d/dz$ is a spatial derivative operator

We will use the notation with a “hat” above the letter to indicate an operator

The most general definition of an operator is an entity that turns one function into another
The particular operator $\hat{H}$ is called the Hamiltonian operator. Just like the classical Hamiltonian function, it is related to the total energy of the system. This Hamiltonian idea extends beyond the specific Schrödinger-equation definition we have so far, which is for single, non-magnetic particles. In general, in non-relativistic quantum mechanics, the Hamiltonian is the operator related to the total energy of the system.
Now we show a simple, important and general relation between the Hamiltonian operator, the wavefunction, and the expectation value of the energy.

To do so, we start by looking at the integral

\[ I = \int \Psi^*(\mathbf{r}, t) \hat{H} \Psi(\mathbf{r}, t) d^3 \mathbf{r} \]

where \( \Psi(\mathbf{r}, t) \) is the wavefunction of some system of interest.
Operators and expectation values

In looking at this integral \( I = \int \Psi^*(r,t) \hat{H} \Psi(r,t) d^3r \)

we will expand the wavefunction \( \Psi(r,t) \) in
the (normalized) energy eigenstates \( \psi_n(r) \)

\[
\Psi(r,t) = \sum_n c_n(t) \psi_n(r)
\]

So

\[
\hat{H} \Psi(r,t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r,t) \right] \Psi(r,t)
\]

\[
= \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r,t) \right] \sum_n c_n(t) \psi_n(r) = \sum_n c_n(t) E_n \psi_n(r)
\]
Operators and expectation values

So the integral becomes

\[
\int \Psi^* (\mathbf{r}, t) \hat{H} \Psi (\mathbf{r}, t) d^3 \mathbf{r} = \int \left[ \sum_m c_m^* (t) \psi_m^* (\mathbf{r}) \right] \times \left[ \sum_n c_n (t) E_n \psi_n (\mathbf{r}) \right] d^3 \mathbf{r}
\]

Because of the orthonormality of the basis functions \( \psi_n (\mathbf{r}) \)
the only terms in the double sum that survive are the ones for which \( n = m \)

so \[
\int \Psi^* (\mathbf{r}, t) \hat{H} \Psi (\mathbf{r}, t) d^3 \mathbf{r} = \sum_n E_n |c_n|^2
\]

But this is just the expectation value of the energy, so

\[
\langle E \rangle = \int \Psi^* (\mathbf{r}, t) \hat{H} \Psi (\mathbf{r}, t) d^3 \mathbf{r}
\]
Benefit of the use of operators

Question:
if we already knew how to calculate $\langle E \rangle$
from $\langle E \rangle = \sum_n E_n P_n = \sum_n E_n |c_n|^2$

why use the new relation?
$\langle E \rangle = \int \Psi^*(\mathbf{r},t) \hat{H} \Psi(\mathbf{r},t) d^3\mathbf{r}$

Answer:
We do not have to solve for the eigenfunctions
of the operator to get the result
4.3 Measurement and expectation values

Slides: Video 4.3.5 Time evolution and the Hamiltonian

Text reference: Quantum Mechanics for Scientists and Engineers

Section 3.11
Taking Schrödinger’s time dependent equation and rewriting it as

and presuming \( \hat{H} \) does not depend explicitly on time, i.e., the potential \( V(\mathbf{r}) \) is constant, could we somehow legally write

\[
\Psi(\mathbf{r}, t_1) = \exp\left(-\frac{i\hat{H}(t_1 - t_0)}{\hbar}\right)\Psi(\mathbf{r}, t_0)
\]
Certainly, if the Hamiltonian operator $\hat{H}$ here was replaced by a constant number we could perform such an integration of

\[
\frac{\partial \Psi (\mathbf{r}, t)}{\partial t} = -\frac{i\hat{H}}{\hbar} \Psi (\mathbf{r}, t)
\]

to get

\[
\Psi (\mathbf{r}, t_1) = \exp \left( -\frac{i\hat{H}(t_1 - t_0)}{\hbar} \right) \Psi (\mathbf{r}, t_0)
\]
Time evolution and the Hamiltonian

If, with some careful definition, it was legal to do this then we would have an operator that gives us the state at time $t_1$ directly from that at time $t_0$.

To think about this “legality” first we note that, because $\hat{H}$ is a linear operator for any number $a$

$$\hat{H} \left[ a \Psi(\mathbf{r},t) \right] = a\hat{H}\Psi(\mathbf{r},t)$$

Since this works for any function $\Psi(\mathbf{r},t)$ we can write as a shorthand

$$\hat{H}a \equiv a\hat{H}$$
Time evolution and the Hamiltonian

Next we have to define what we mean by an operator raised to a power.

By $\hat{H}^2$ we mean $\hat{H}^2 \Psi(r,t) = \hat{H} \left[ \hat{H} \Psi(r,t) \right]$

Specifically, for example, for the energy eigenfunction $\psi_n(r)$

$\hat{H}^2 \psi_n(r) = \hat{H} \left[ \hat{H} \psi_n(r) \right] = \hat{H} \left[ E_n \psi_n(r) \right] = E_n \hat{H} \psi_n(r) = E_n^2 \psi_n(r)$

We can proceed inductively to define all higher powers

$\hat{H}^{m+1} \equiv \hat{H} \left[ \hat{H}^m \right]$

which will give, for the an energy eigenfunction

$\hat{H}^m \psi_n(r) = E_n^m \psi_n(r)$
Time evolution and the Hamiltonian

Now let us look at the time evolution of some wavefunction $\Psi(r, t)$ between times $t_0$ and $t_1$.

Suppose the wavefunction at time $t_0$ is $\psi(r)$ which we expand in the energy eigenfunctions $\psi_n(r)$ as

$$\psi(r) = \sum_n a_n \psi_n(r)$$

Then we know

multiplying by the complex exponential factors for the time-evolution of each basis function

$$\Psi(r, t_1) = \sum_n a_n \exp\left[-\frac{iE_n(t_1 - t_0)}{\hbar}\right] \psi_n(r)$$
Time evolution and the Hamiltonian

In

\[ \Psi(\mathbf{r}, t_1) = \sum_n a_n \exp \left[ -\frac{iE_n(t_1 - t_0)}{\hbar} \right] \psi_n(\mathbf{r}) \]

noting that \( \exp(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots \)

we can write the exponentials as power series

so

\[ \Psi(\mathbf{r}, t_1) = \sum_n a_n \left[ 1 + \left( -\frac{iE_n(t_1 - t_0)}{\hbar} \right) + \frac{1}{2!} \left( -\frac{iE_n(t_1 - t_0)}{\hbar} \right)^2 + \cdots \right] \psi_n(\mathbf{r}) \]
Time evolution and the Hamiltonian

In

\[ \Psi(r,t_1) = \sum_n a_n \left[ 1 + \left( -\frac{iE_n(t_1-t_0)}{\hbar} \right) + \frac{1}{2!} \left( -\frac{iE_n(t_1-t_0)}{\hbar} \right)^2 + \cdots \right] \psi_n(r) \]

because we showed that \( \hat{H}^m \psi_n(r) = E_n^m \psi_n(r) \)
we can substitute to obtain

\[ \Psi(r,t_1) = \sum_n a_n \left[ 1 + \left( -\frac{i\hat{H}(t_1-t_0)}{\hbar} \right) + \frac{1}{2!} \left( -\frac{i\hat{H}(t_1-t_0)}{\hbar} \right)^2 + \cdots \right] \psi_n(r) \]
Time evolution and the Hamiltonian

With

\[ \Psi(r,t_1) = \sum_n a_n \left[ 1 + \left( -\frac{i\hat{H}(t_1 - t_0)}{\hbar} \right) + \frac{1}{2!} \left( -\frac{i\hat{H}(t_1 - t_0)}{\hbar} \right)^2 + \cdots \right] \psi_n(r) \]

because the operator \( \hat{H} \) and all its powers commute with scalar quantities (numbers) we can rewrite

\[ \Psi(r,t_1) = \left[ 1 + \left( -\frac{i\hat{H}(t_1 - t_0)}{\hbar} \right) + \frac{1}{2!} \left( -\frac{i\hat{H}(t_1 - t_0)}{\hbar} \right)^2 + \cdots \right] \sum_n a_n \psi_n(r) \]

\[ = \left[ 1 + \left( -\frac{i\hat{H}(t_1 - t_0)}{\hbar} \right) + \frac{1}{2!} \left( -\frac{i\hat{H}(t_1 - t_0)}{\hbar} \right)^2 + \cdots \right] \Psi(r,t_0) \]
Time evolution and the Hamiltonian

So, provided we define the exponential of the operator in terms of a power series, i.e.,

\[
\exp\left[-\frac{i\hat{H}(t_1-t_0)}{\hbar}\right] \equiv 1 + \left(-\frac{i\hat{H}(t_1-t_0)}{\hbar}\right) + \frac{1}{2!}\left(-\frac{i\hat{H}(t_1-t_0)}{\hbar}\right)^2 + \ldots
\]

then we can write our preceding expression as

\[\Psi(r, t_1) = \exp\left(-\frac{i\hat{H}(t_1-t_0)}{\hbar}\right)\Psi(r, t_0)\]
Time evolution and the Hamiltonian

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 $t_1$

$$\Psi(r, t_1) = \exp\left(-\frac{i\hat{H}(t_1 - t_0)}{\hbar}\right)\Psi(r, t_0)$$