

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





Measurement and expectation values



Quantum-mechanical measurement

Quantum mechanics for scientists and engineers

David Miller

Probabilities and expansion coefficients

Suppose we take some (normalized) quantum mechanical wave function $\Psi(\mathbf{r}, t)$

and expand it in some complete orthonormal set of spatial functions $\psi_n(\mathbf{r})$

At least if we allow the expansion coefficients c_n to vary in time

we know we can always do this

$$\Psi(\mathbf{r}, t) = \sum_n c_n(t) \psi_n(\mathbf{r})$$

Probabilities and expansion coefficients

Then the fact that $\Psi(\mathbf{r}, t)$ is normalized means

we know the answer for the normalization integral

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

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 $|c_n(t)|^2$

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

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

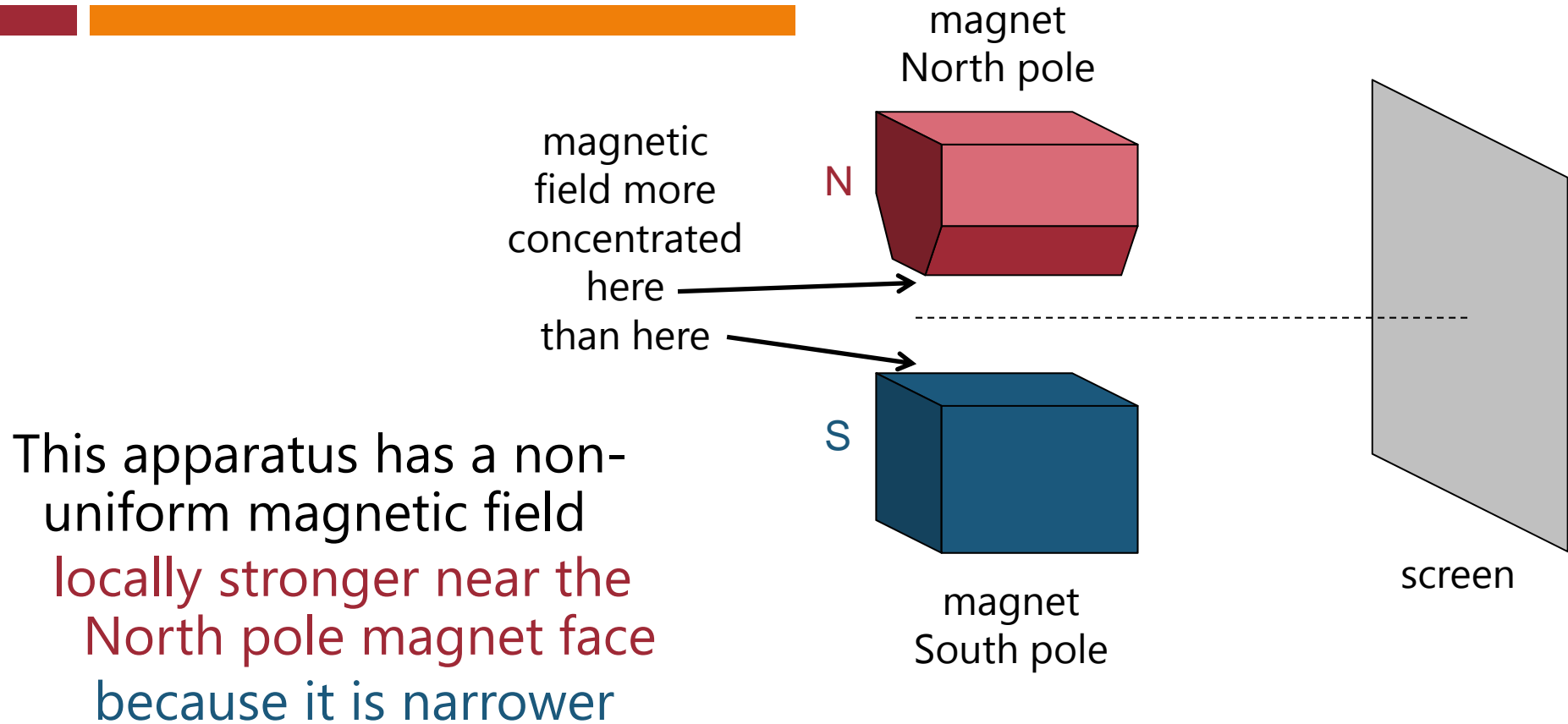
where we use the result that the average in a Poisson statistical distribution is just the parameter N

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

Stern-Gerlach experiment



Stern-Gerlach experiment

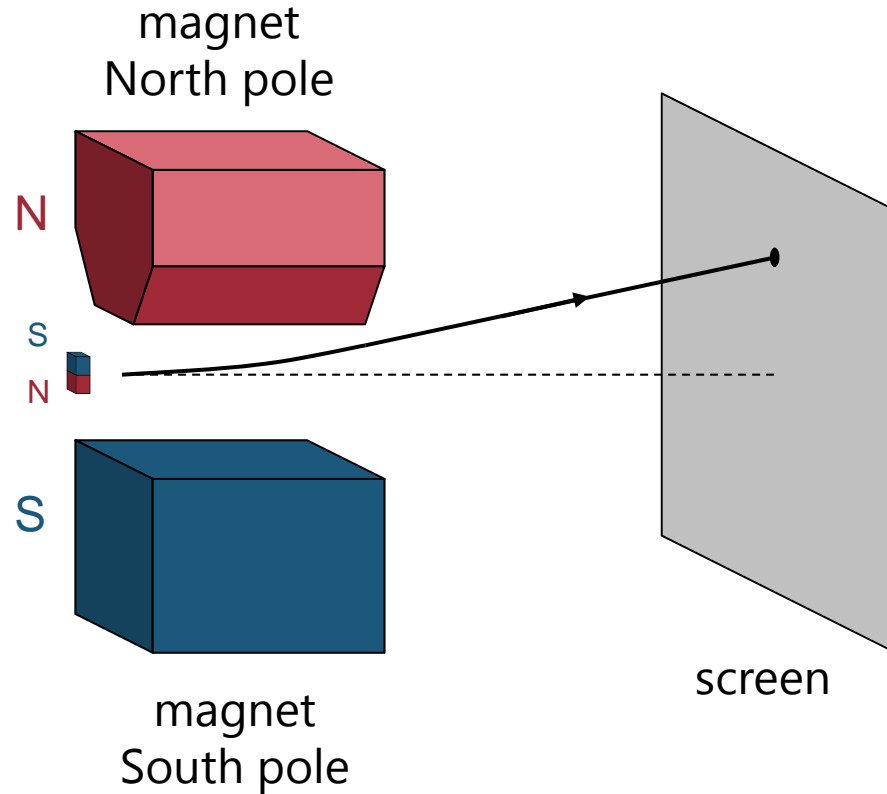
Imagine firing some small magnets

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



Stern-Gerlach experiment

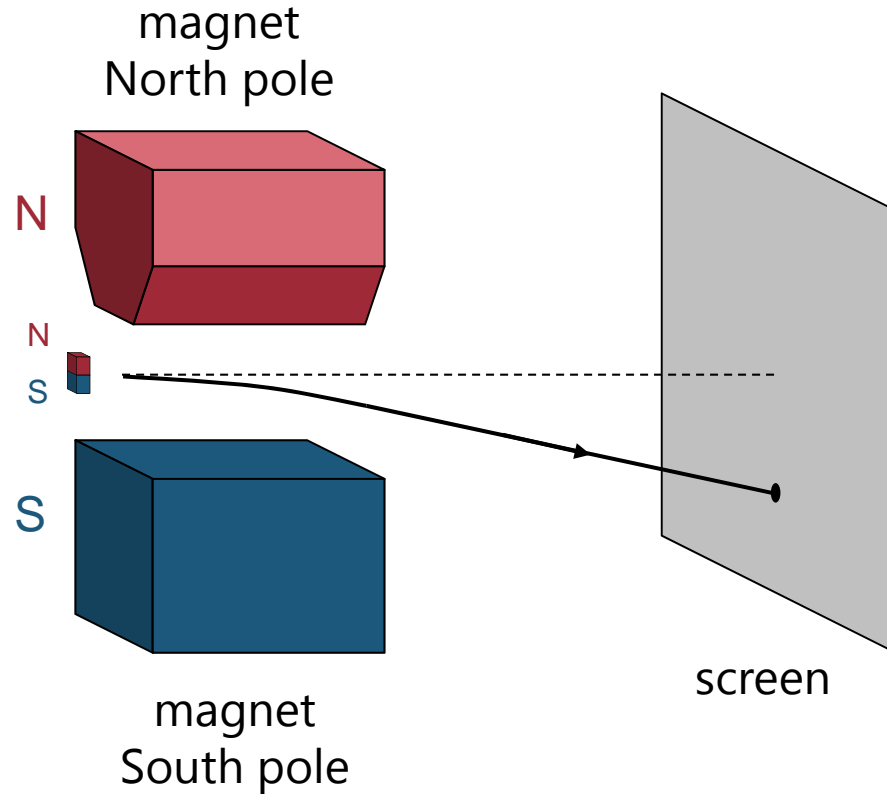
Imagine firing some small magnets

initially along the dashed line

Because the magnetic field is non-uniform

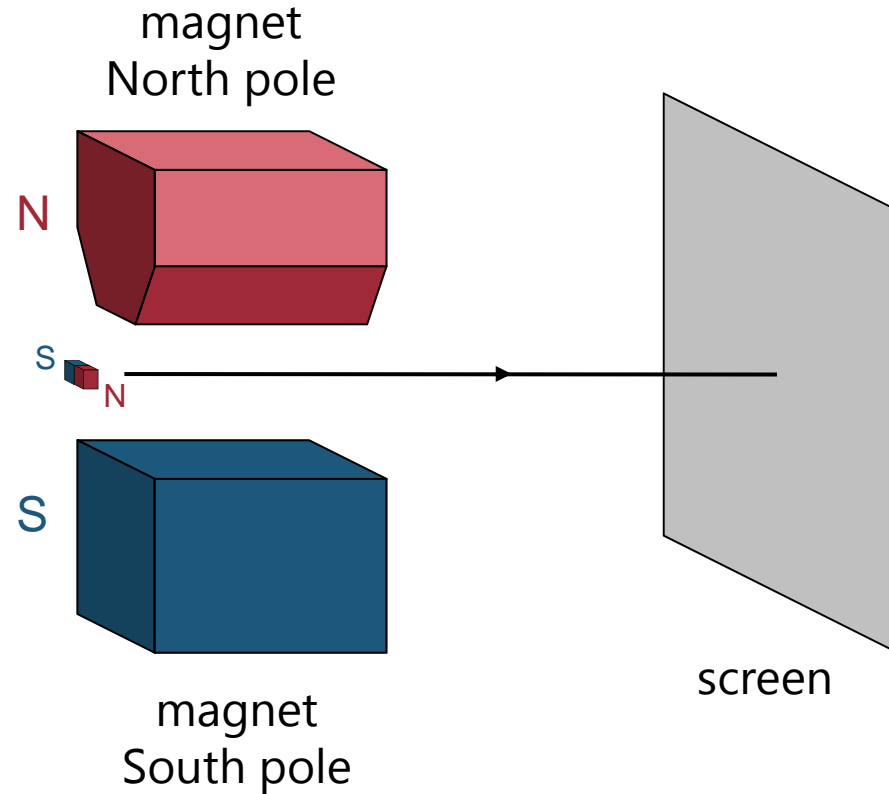
stronger near the North pole than near the South pole

a vertical magnet will be deflected up or down



Stern-Gerlach experiment

A horizontally-oriented magnet
will not be deflected



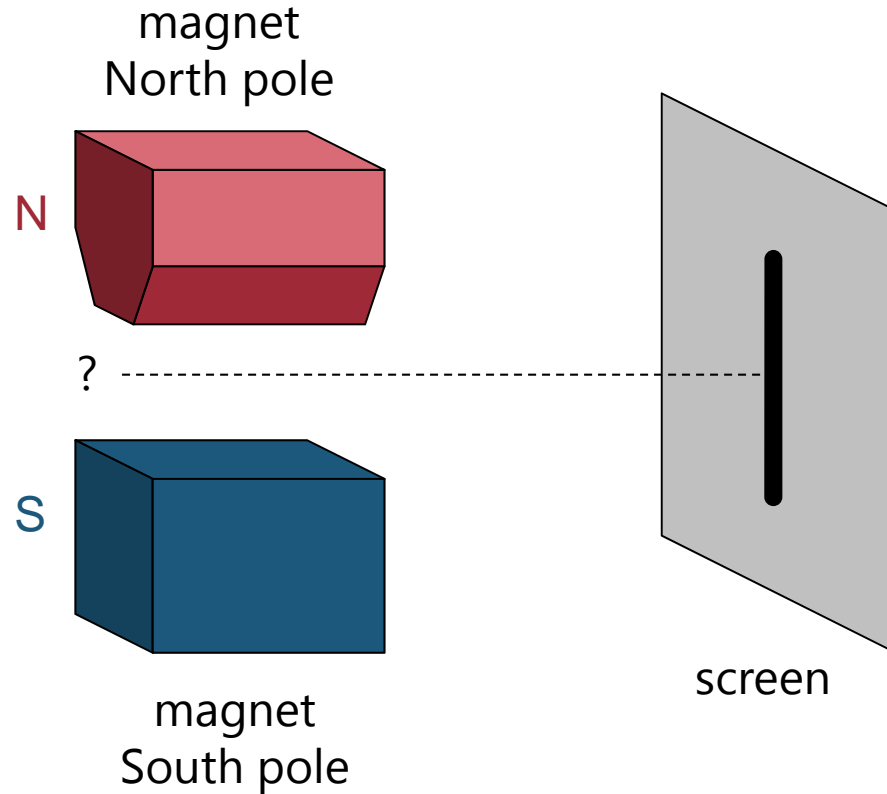
Stern-Gerlach experiment

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!

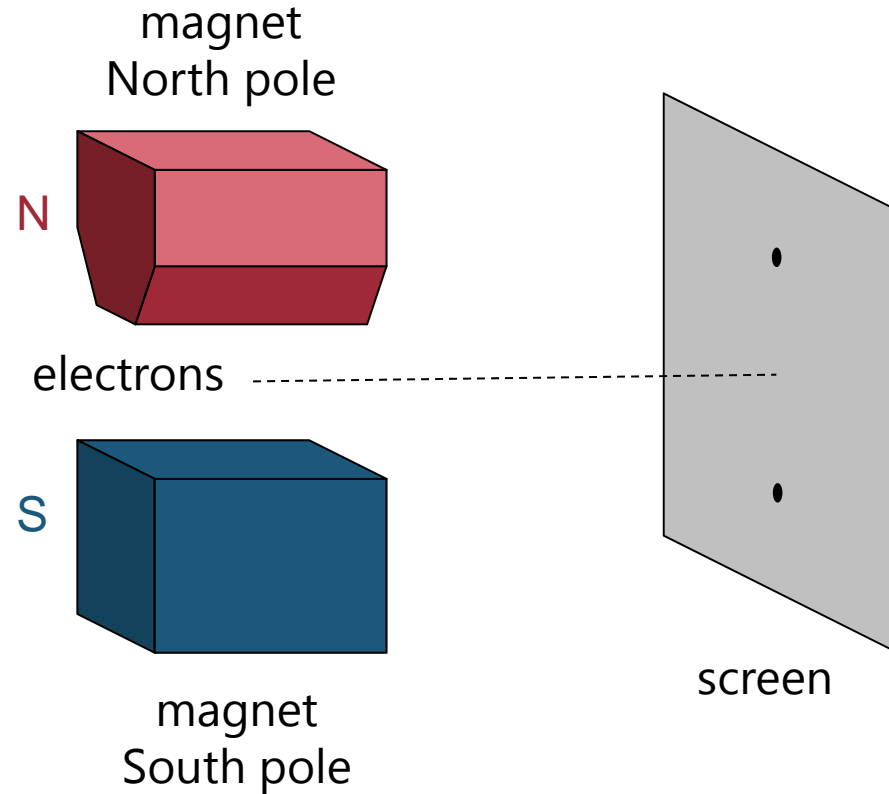
"Explanation"

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



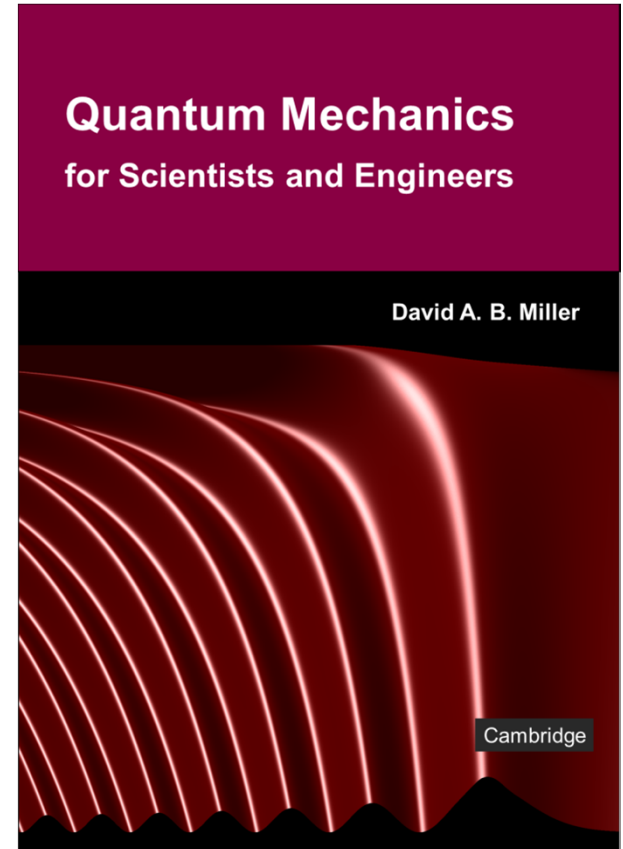


4.3 Measurement and expectation values

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

Hamiltonian operator

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 $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}, t)$

so we can write the Schrödinger equations as

$$\hat{H}\psi(\mathbf{r}) = E\psi(\mathbf{r}) \text{ and } \hat{H}\Psi(\mathbf{r}, t) = i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t}$$

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

Hamiltonian operator

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

Operators and expectation values

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

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

$$\Psi(\mathbf{r}, t) = \sum_n c_n(t) \psi_n(\mathbf{r})$$

So

$$\begin{aligned} \hat{H} \Psi(\mathbf{r}, t) &= \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) \right] \Psi(\mathbf{r}, t) \\ &= \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t) \right] \sum_n c_n(t) \psi_n(\mathbf{r}) = \sum_n c_n(t) E_n \psi_n(\mathbf{r}) \end{aligned}$$

Operators and expectation values

So the integral becomes

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

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

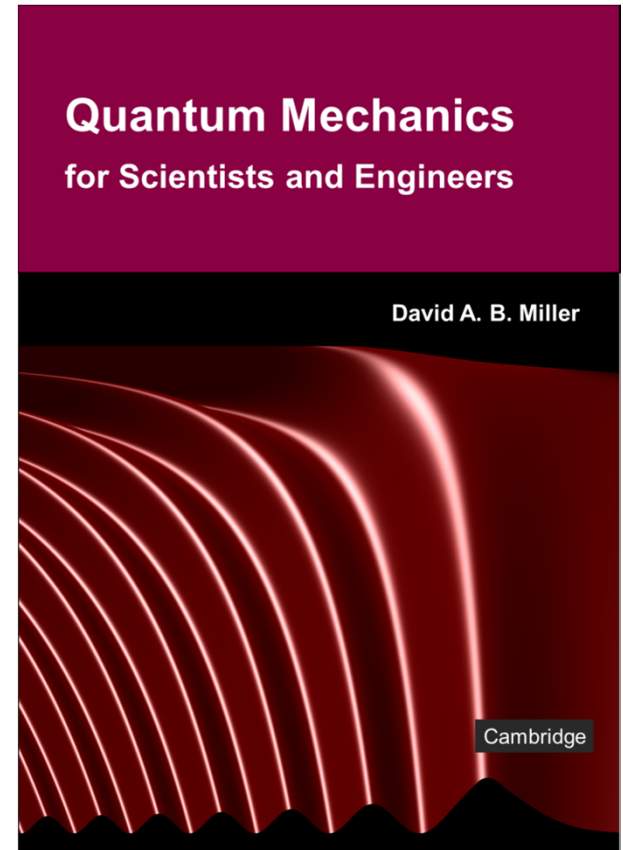


4.3 Measurement and expectation values

Slides: Video 4.3.5 Time evolution and the Hamiltonian

Text reference: Quantum Mechanics for Scientists and Engineers

Section 3.11





Measurement and expectation values



Time evolution and the Hamiltonian

Quantum mechanics for scientists and engineers

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Time evolution and the Hamiltonian

Taking Schrödinger's time dependent equation

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

and rewriting it as

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

and presuming \hat{H} does not depend explicitly on time

i.e., the potential $V(\mathbf{r})$ is constant

could we somehow legally write

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

Time evolution and the Hamiltonian

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

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

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 $\hat{H}^2\Psi(\mathbf{r},t) = \hat{H}[\hat{H}\Psi(\mathbf{r},t)]$

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

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

We can proceed inductively to define all higher powers

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

which will give, for the an energy eigenfunction

$$\hat{H}^m\psi_n(\mathbf{r}) = E_n^m\psi_n(\mathbf{r})$$

Time evolution and the Hamiltonian

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

Suppose the wavefunction at time t_0 is $\psi(\mathbf{r})$

which we expand in the energy eigenfunctions $\psi_n(\mathbf{r})$

as
$$\psi(\mathbf{r}) = \sum_n a_n \psi_n(\mathbf{r})$$

Then we know

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

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

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 $\exp(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots$

we can write the exponentials as power series

so

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

Time evolution and the Hamiltonian

In

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

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

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

Time evolution and the Hamiltonian

With

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

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

$$\begin{aligned} \Psi(\mathbf{r}, t_1) &= \left[1 + \left(-\frac{i\hat{H}(t_1 - t_0)}{\hbar} \right) + \frac{1}{2!} \left(-\frac{i\hat{H}(t_1 - t_0)}{\hbar} \right)^2 + \dots \right] \sum_n a_n \psi_n(\mathbf{r}) \\ &= \left[1 + \left(-\frac{i\hat{H}(t_1 - t_0)}{\hbar} \right) + \frac{1}{2!} \left(-\frac{i\hat{H}(t_1 - t_0)}{\hbar} \right)^2 + \dots \right] \Psi(\mathbf{r}, t_0) \end{aligned}$$

Time evolution and the Hamiltonian

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

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

then we can write our preceding expression as

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

Time evolution and the Hamiltonian

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

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

