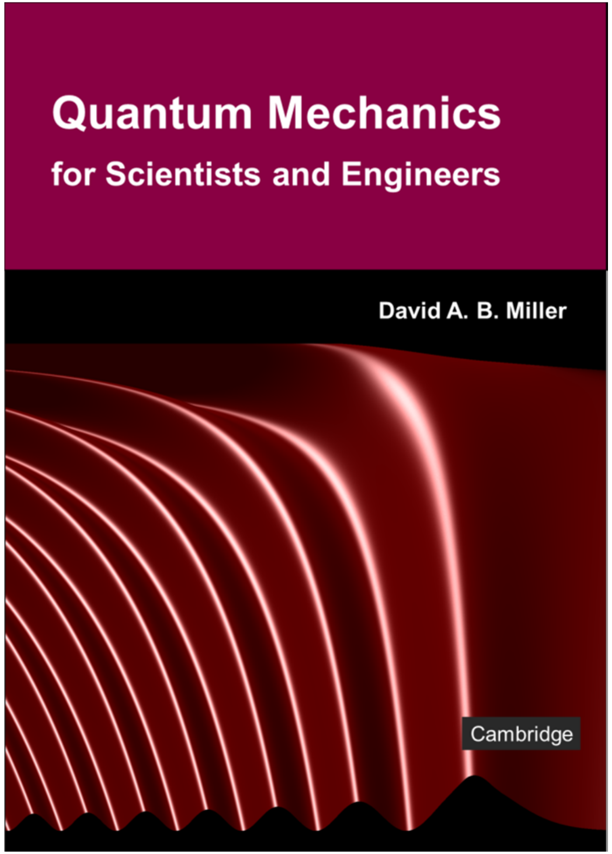
4.3 Measurement and expectation values

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

$\hat{H}\psi(\mathbf{r}) = E\psi(\mathbf{r})$ 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

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

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

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

$$\boxed{\langle E\rangle = \int \Psi^*(\mathbf{r},t)\hat{H}\Psi(\mathbf{r},t)d^3\mathbf{r}}$$

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