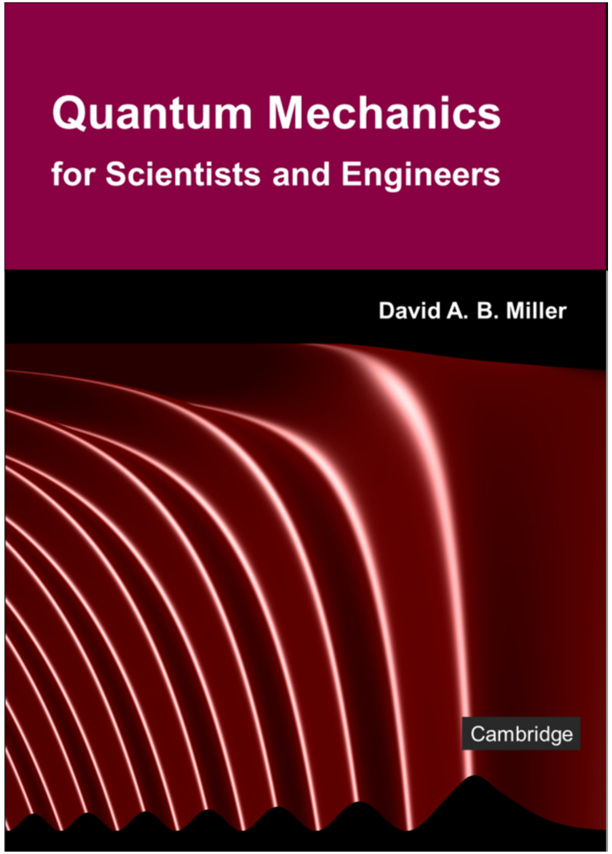
4.3 Measurement and expectation values

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

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

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

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

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

We can proceed inductively to define all higher powers

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

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

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

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

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

we can substitute to obtain

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

Time evolution and the Hamiltonian

With

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

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

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

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

Time evolution and the Hamiltonian

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

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

then we can write our preceding expression as

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

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

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