

EE 236  
9/3/2004  
①

Hamiltonians  
Particle in a 1-D box  
expectation values

In the last lecture, we showed that if we have a QM system with a finite number of states, we can define Hermitian operators over those states, and associate the concept of "measurement" of some value with one of those Hermitian operators.

If we have a complete, orthonormal set of eigenstates  $|a_n\rangle$  (and any nonsingular, Hermitian operator with all discrete eigenvalues will give us such a set)  $A$  we can express any state of the system as a vector (of numbers)  $C_n$

$$\psi = \sum C_n |a_n\rangle$$

and we can also use the set to express any other operator  $\hat{B}$ . For example:

$$|\phi\rangle = \hat{B} |\psi\rangle$$

using the identity,  $\hat{I} = \sum_n |a_n\rangle \langle a_n|$

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$$|\phi\rangle = \sum_n \sum_m |a_n\rangle \{ \langle a_n | \hat{B} | a_m \rangle \} \langle a_m | \psi \rangle$$

$$|\phi\rangle = \sum_n \sum_m |a_n\rangle \langle a_m | \{ \langle a_n | \hat{B} | a_m \rangle \} |\psi\rangle$$

$$\langle a_n | \phi \rangle = \sum_m \{ \langle a_n | \hat{B} | a_m \rangle \} \langle a_m | \psi \rangle$$

but this is just the rule for  
matrix multiplication with

$$[\hat{B}]_{mn} = \langle a_n | \hat{B} | a_m \rangle$$

$$+ [\psi]_m = \langle a_m | \psi \rangle$$

$$+ [\phi]_n = \langle a_n | \phi \rangle$$

So choosing a basis observable  
operator  $\hat{A}$  let us describe  
all operators in the space as  
matrices, and all states of the  
system as vectors

(but they will change if  
we pick another operator  $\hat{B}$   
as our basis operator)

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The most important operator is often the Hamiltonian operator, where

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle$$

where  $|\Psi(t)\rangle$  represents an arbitrary state of the system at time  $t$

the eigenstates of  $\hat{H}$  are the stationary states

$$\hat{H} |\phi_n\rangle = E_n |\phi_n\rangle$$

$$i\hbar \frac{\partial}{\partial t} |\phi_n(t)\rangle = E_n |\phi_n(t)\rangle$$

$$|\phi_n(t)\rangle = e^{-i\omega_n t} |\phi_n(0)\rangle$$

$$\text{where } \hbar\omega_n = E_n$$

so they just change phase in time

this allows us to solve the time dependance of systems:

$$|\Psi(t)\rangle = \sum_n |\phi_n\rangle \langle \phi_n | \Psi \rangle$$

$$|\Psi(t=0)\rangle = \sum_n \langle \phi_n | \Psi \rangle |\phi_n\rangle$$

$$|\Psi(t)\rangle = \sum_n \langle \phi_n | \Psi \rangle e^{-i\omega_n t} |\phi_n\rangle$$

let's take as an example, a charged particle in a 1-D box (we will ignore spin for now)

The possible states of the system are the functions of  $x$  and independent variable over the interval  $-a < x < a$  where  $\psi(x)$  is continuous & differentiable, and  $\psi(-a) = 0$  and  $\psi(a) = 0$

$|\psi\rangle$  - function  $\psi(x)$ ; the inner-product will be defined as

$$\langle \phi | \psi \rangle = \int_{-a}^a \phi^*(x) \psi(x) dx$$

Operators are any mapping from  $f(x) \rightarrow g(x)$  where both  $f(x)$  &  $g(x)$  satisfy the above

The Hamiltonian operator is the operator given by the Schrödinger equation

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + \cancel{V(x,t)} \right]$$

where  $V(x,t) = 0$   $\nabla^2 \rightarrow \frac{\partial^2}{\partial x^2}$

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$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

To find the eigenstates and eigenvalues of  $\hat{H}$ , we note that

$$\hat{H} |\phi_n\rangle = E_n |\phi_n\rangle$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \phi_n(x) = E_n \phi_n(x)$$

The solutions to this equation are  $\sin(Kx)$  &  $\cos(Kx)$

$$\frac{\hbar^2}{2m} K^2 \sin(Kx) = E_n \sin(Kx)$$

$$\frac{\hbar^2}{2m} K^2 \cos(Kx) = E_n \cos(Kx)$$

$$E_n = \frac{\hbar^2 K^2}{2m}$$

Using the B.C.'s we have

$$\cos(Ka) = 0 \Rightarrow Ka = \pi/2 + n\pi$$

$$\text{or } \sin(Ka) = 0 \quad Ka = n\pi$$

So the energy eigenstates are

$$|\phi_n\rangle \rightarrow \phi_{no}(x) = C_{no} \sin\left[\left(\frac{\pi}{2} + n\pi\right) \frac{x}{a}\right]$$

$$\text{or } \phi_{ne}(x) = C_{ne} \cos\left[n\pi \frac{x}{a}\right]$$

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Since the inner product is

$$\langle \phi | \psi \rangle = \int_{-a}^a \phi^*(x) \psi(x) dx$$

$$\langle \phi_{n0} | \phi_{n0} \rangle = \int_{-a}^a |C_{n0}|^2 \sin^2\left(\frac{\pi}{2} + n\pi \frac{x}{a}\right)$$

so to normalize we want

$$1 = 2a |C_{n0}|^2 \frac{1}{2}$$

$$|C_{n0}|^2 = \frac{1}{2a}$$

and we arbitrarily choose the phase

$$C_{n0} = \frac{1}{\sqrt{2a}}$$

Eigenvalues

$$\frac{\hbar^2}{2m} \left(\frac{\pi}{2} + m\pi\right)^2$$

$$\frac{\hbar^2}{2m} (m\pi)^2$$

Eigenstates

$$\frac{1}{\sqrt{2a}} \sin\left[\left(\frac{\pi}{2} + n\pi\right) \frac{x}{a}\right]$$

$$\frac{1}{\sqrt{2a}} \cos\left[(n\pi) \frac{x}{a}\right]$$

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Now lets "measure" where the electron is.

The operator corresponding to the measurement of  $x$  is to multiply the wavefunction by  $x$

$$\hat{X} \rightarrow x_0$$

The eigenvalues of  $X$  can be found by

$$\hat{X} f(x) = x_n f(x)$$

$$|x_n\rangle \Rightarrow \delta(x-x_n)$$

The probability of measuring any particular value of  $x_0$  is

$$|\langle x_n | \psi \rangle|^2 = \left| \int_{-a}^a \delta(x-x_n) \psi(x) dx \right|^2$$

and the particle will be in a  $\delta(x)$  state after the measurement.

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This corresponds to a probability distribution

$$P(x, t) = \psi^*(x, t) \psi(x, t)$$

For a time  $t$  and a measurement of the position  $x$  however if the position of  $x$  is measured, it will perturb the system.

To correspond to a probability distribution, we need the sum of all possible outcomes to have a probability 1

$$\int_{-a}^a P(x, t) = 1$$

but this just gives us

$$\int_{-a}^a \psi^*(x, t) \psi(x, t) dx = 1$$

which is the same as our normalization condition

Notice that to refer to our classical intuition, we use the term "probability amplitude" for something which has nothing to do with probabilities until a measurement is made, and then the distribution becomes irrelevant!

I think a better way to look at it is that electrons are something like a lump of jelly which undulates & moves & spreads out

- It does not have a probability of being in a number of places it is spread out in space.

In 3-D, the situation is the same, except the Hamiltonian is

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r,t) \right] \psi = i\hbar \frac{\partial \psi}{\partial t}$$

and the inner product is  $\langle \phi | \psi \rangle = \iiint_{\text{Volume}} \phi^*(\vec{r}) \psi d\vec{r}$

One thing that we can depend on in quantum mechanics is that no matter how strange things get, they will become familiar in the classical limit.

One way that we can get back to the familiar is through concepts such as the expectation value of observables.

If we take an observable associated with an operator  $\hat{A}$ , and expand an arbitrary state of the system over the eigenstates of  $\hat{A}$

$$|\psi\rangle = \sum_n c_n |A_n\rangle$$

the probability of "measuring" the value  $a_n$  is

$$| \langle A_n | \psi \rangle |^2$$

so we can define an "expectation value" for the observable  $A$

$$\sum_n a_n P(a_n)$$

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$$\begin{aligned}
 \text{Expectation}(A) &= \sum_n a_n P(a_n) \\
 &= \sum_n a_n |\langle A_n | \psi \rangle|^2 \\
 &= \sum_n \langle \psi | A_n \rangle a_n \langle A_n | \psi \rangle
 \end{aligned}$$

but if we look at the operator

$$\sum_n |A_n\rangle a_n \langle A_n|$$

we see that if we apply it to any eigenstate of  $\hat{A}$ :  $|A_n\rangle$  we get  $a_n |A_n\rangle \rightarrow$  this is just the operator  $\hat{A}$ !

$$\begin{aligned}
 \text{Expectation}(A) &= \langle \psi | \hat{A} | \psi \rangle \\
 \rightarrow \text{if the system is in state } \hat{A}
 \end{aligned}$$

In many cases we will consider, there will be many similar Q.M. systems in our experiment, so that the expectation values will come out to be average values (over a volume of material, for example)