Properties of Operators and Eigenfunctions

1 Properties of Operators

Linear Operators:

An operator $\hat{\mathcal{O}}$ is called "Linear Operator" if

$$\hat{\mathcal{O}}\left[\psi_1(x)+\psi_2(x)\right]=\hat{\mathcal{O}}\psi_1(x)+\hat{\mathcal{O}}\psi_2(x).$$

For example, the position operator $\hat{X}$ that we defined is a linear operator. It is easy to see that

$$\begin{aligned}\hat{X}\left[\psi_1(x)+\psi_2(x)\right] &= x\left[\psi_1(x)+\psi_2(x)\right]\\ &= x\psi_1(x)+x\psi_2(x)=\hat{X}\psi_1(x)+\hat{X}\psi_2(x).\end{aligned}$$

You can also verify that the momentum operator $\hat{P}=-i\hbar d/dx$ and kinetic energy operator $(\hat{P})^2/2m=-[\hbar^2/(2m)]d^2/dx^2$ are linear operators. Let us consider a simple example of a non-linear operator. Let us define "$\hat{S}$" operator which gives the sine of any function on which it acts:

$$\hat{S}\psi(x)=\sin(\psi(x)).$$

Obviously

$$\hat{S}\left[\psi_1(x)+\psi_2(x)\right]\neq\hat{S}\psi_1(x)+\hat{S}\psi_2(x).$$

All the operators in quantum mechanics, which represent physical observables, are linear operators.

2 Notion of "dot product" of two functions

You all have heard of "dot product" of two vectors. For two vectors in three dimensions, $\vec{A}$ and $\vec{B}$, the dot product is defined to be

$$\vec{A}\cdot\vec{B}=A_xB_x+A_yB_y+A_zB_z.$$

Sometimes we use matrix notation to write vectors and their dot products. If the vectors are represented by column matrices

$$\vec{A} = \begin{bmatrix} A_x \\ A_y \\ A_z \end{bmatrix} \quad \text{and} \quad \vec{B} = \begin{bmatrix} B_x \\ B_y \\ B_z \end{bmatrix},$$

the dot product is the matrix product

$$\begin{bmatrix} A_x & A_y & A_z \end{bmatrix} \begin{bmatrix} B_x \\ B_y \\ B_z \end{bmatrix}.$$

If we calculate the "norm-square" of a vector by defining its dot product with itself

$$|A|^2 = \begin{bmatrix} A_x & A_y & A_z \end{bmatrix} \begin{bmatrix} A_x \\ A_y \\ A_z \end{bmatrix}.$$

We have already defined the norm of a wave function $\psi(x)$ as

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-\infty}^{\infty} \psi^*(x)\psi(x) dx.$$

We use this as a template to define the **dot product** of two wave functions $\psi_1(x)$ and $\psi_2(x)$ as

$$\int_{-\infty}^{\infty} \psi_1^*(x)\psi_2(x) dx.$$

Note that we used the same definition to define the **orthogonality** of eigenfunctions in earlier lecture.

In the case of three dimensional vectors, we have $\vec{A} \cdot \vec{B} = \vec{B} \cdot \vec{A}$. That is, the dot product is **commutative**. Because the wave functions $\psi_1(x)$ and $\psi_2(x)$ are, in general, complex. So the order of multiplication matters because

$$\int_{-\infty}^{\infty} \psi_1^*(x)\psi_2(x) dx \neq \int_{-\infty}^{\infty} \psi_2^*(x)\psi_1(x) dx.$$

In general the (12) dot product is the complex conjugate of the (21) dot product. In the special case when both the wave functions $\psi_1(x)$ and $\psi_2(x)$ are real, the two dot products are the same.

3 Hermitian Operators

In quantum mechanics, all physical observables are associated with operators. When this was mentioned in an earlier lecture, the question was raised "Why should the eigenvalues of these operators be real?" The answer to that question is: **All physical observables are associated with Hermitian Operators.** It can be proved that **Hermitian** operators have only real (not necessarily positive) eigenvalues.

What is a "Hermitian" operator? Consider an operator $\hat{\mathcal{O}}$. It acts on a wave function $\psi_1(x)$ and gives another function $\hat{\mathcal{O}}\psi_1(x)$. Now consider the dot product of this fuction with another wave function $\psi_2(x)$

$$\int_{-\infty}^{\infty} \psi_2^*(x)\hat{\mathcal{O}}\psi_1(x)dx \equiv \mathcal{O}_{21}.$$

The number $\mathcal{O}_{21}$ is called the **matrix element** of the operator $\mathcal{O}$ between the wave functions $\psi_2(x)$ and $\psi_1(x)$. In a similar way, we can define matrix elements $\mathcal{O}_{ij}$ as

$$\int_{-\infty}^{\infty} \psi_i^*(x)\hat{\mathcal{O}}\psi_j(x)dx \equiv \mathcal{O}_{ij}.$$

That is, we think of the operator $\hat{\mathcal{O}}$ as **infinite dimensional matrix**. When $\psi_i(x) = \psi_j(x)$, we get the **diagonal elements** of this matrix. When $\psi_i(x) \neq \psi_j(x)$, we get the **off-diagonal elements** of the matrix.

An operator $\hat{\mathcal{O}}$ is called a **Hermitian operator** if the matrix elements satisfy the condition

$$\mathcal{O}_{ji}^* = \mathcal{O}_{ij}, \quad \text{for every } i \text{ and } j.$$

For $i = j$, this equation reduces to $\mathcal{O}_{ii}^* = \mathcal{O}_{ii}$, which means the **diagonal elements of a Hermitian matrix are real**. The pairs of off-diagonal elements $\mathcal{O}_{ij}$ and $\mathcal{O}_{ji}$ are complex conjugates of each other.

In matrix notation, I guess you are familiar with the notion of **transpose**. If A is a matrix with elements A_{ij}, then A^T is a matrix with elements $(A^T)_{ij} = A_{ji}$. In constructing the transposed matrix, we leave the diagonal elements alone and interchange the pair wise off-diagonal elements $(ij) \leftrightarrow (ji)$. A matrix is called a **symmetric matrix** if $A^T = A$. This notion can be extended to Hermitian matrices. If B is a matrix, we define its **Hermitian conjugate**, denoted by $B^\dagger$, as

$$(B^\dagger)_{ij} = B_{ji}^*.$$

A matrix is Hermitian, if it is equal to its Hermitian Conjugate. That is, if $B^\dagger = B$. You note that this condition is the same as the one given above for the Hermiticity of $\mathcal{O}$. You can verify that the position operator, the momentum operator and the Hamiltonian are all Hermitian. As mentioned above, it can be shown that **Hermitian operators have real eigenvalues**.

4 Commutator of two Operators

Consider two operators $\hat{A}$ and $\hat{B}$. Given these two operators, we can consider two possibilities. One possibility is, first $\hat{A}$ acts on a wave function and then $\hat{B}$ acts on the result. We call the net result $\hat{B}\hat{A}\psi(x)$. The other possibility is, first $\hat{B}$ acts on $\psi(x)$ and then $\hat{A}$ acts on the result. The net result here is denoted $\hat{A}\hat{B}\psi(x)$. In general

$$\hat{A}\hat{B}\psi(x) \neq \hat{B}\hat{A}\psi(x),$$

So

$$\hat{A}\hat{B}\psi(x) - \hat{B}\hat{A}\psi(x) = \left(\hat{A}\hat{B} - \hat{B}\hat{A}\right)\psi(x) \neq 0.$$

We define the **commutator** of two operators as

$$\left(\hat{A}\hat{B} - \hat{B}\hat{A}\right) \equiv [\hat{A}, \hat{B}].$$

For two arbitrary operators, $\hat{A}$ and $\hat{B}$, their **commutator is not zero**. Take $\hat{A} = \hat{X}$ and $\hat{B} = \hat{P}$ and calculate $\hat{X}\hat{P}\psi(x) - \hat{P}\hat{X}\psi(x)$, where $\psi(x)$ is any arbitrary wave function. You will find

$$[\hat{X}, \hat{P}]\,\psi(x) = i\hbar\psi(x).$$

In operator language, this is stated as

$$[\hat{X}, \hat{P}] = i\hbar I,$$

where I is **identity operator** (it leaves $\psi(x)$ untouched). It can be shown that the above commutator relation leads to Heisenberg Uncertainty relation $\Delta x \Delta p \geq \hbar/2$.

Two operators are said to commute if

$$\hat{A}\hat{B}\psi(x) = \hat{B}\hat{A}\psi(x),$$

for every $\psi(x)$. In operator language, it is stated as

$$[\hat{A}, \hat{B}] = 0.$$

An important theorem states that, **two commuting operators have simultaneous eigenfunctions**. That is, there is a single set of eigenfunctions $\phi_n(x)$, which are simultaneously eigenfunctions of $\hat{A}$ and of $\hat{B}$.

5 Connecting Calculations to Measurements

So far, we have given a lot of definitions and prescriptions to calculate expectation values and uncertainties. But, an important question we must address is **How do we relate these calculations to measurements?**

To give a better physical picture, we illustrate this issue using the example of **Hamiltonian operator.** We consider an particle of mass m, bound a potential well $V(x)$. We will not explicitly specify the potential but assume that it is well behaved. Given the potential, we can write the corresponding time independent Schroedinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\phi_n(x)}{dx^2} + V(x)\phi_n(x) = E_n\phi_n(x).$$

Here, I assumed that, the potential has a set of **orthonormal** energy eigenfunctions $\phi_n(x)$, with the corresponding energy eigenvalues E_n. We saw earlier if the wave function of the particle $\psi(x) = \phi_n(x)$, then a measurement of energy of the particle will give answer E_n. We also saw that, a particle kept in such a state will remain there for all time, until it is disturbed.

What if $\psi(x) \neq \phi_n(x)$ but, in stead, is a linear combination of a number of ϕ_ns? Suppose

$$\psi(x) = \sum_n C_n\phi_n(x),$$

where C_ns are constants (they can be either real or complex). Also, the sum can have either a finite number of terms or an infinite number of terms. If the particle is in a state described by the above $\psi(x)$, what happens when we measure the energy?

Fundamental Assumption on Measurement: A measuring apparatus, which measures the energy of a particle, **forces the wave function of the particle to one of the energy eigenfunctions**! This also goes under the name **Collapse of the wave function**. It is the least understood part of quantum mechanics. It is a topic of active research and there is some recent progress. We make this assumption because it works. We are able to explain all the experimental results based on this assumption. Let us accept this assumption and apply it to the above wave function.

Initially, the wave function of the particle is $\psi(x)$. The act of measuring its energy will force it into an energy eigenfunction. But, that can be any one of the eigenfunctions in the sum $\sum_n C_n\phi_n(x)$. Suppose, our measurement gives the result E_m, which means that the measurement forced it into the state $\phi_m(x)$. The question we ask is the following: Suppose we had a very large number N of identical particles, each bound in the same potential $V(x)$ that we considered earlier. We make an energy measurement on each of these particles and we get the answer to be E_m in $(p_m\,N)$ of the cases. **Can we predict the value of the probability p_m?** Answer is: YES!!

In the previous lecture, we considered the normalization of $\psi(x) = \sum_n C_n\phi_n(x)$. Let us consider it in detail.

$$\begin{aligned}
\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx &= \int_{-\infty}^{\infty} \sum_m C_m^*\phi_m^*(x) \sum_n C_n\phi_n(x)dx \\
&= \sum_m \sum_n C_m^* C_n \int_{-\infty}^{\infty} \phi_m^*(x)\phi_n(x)dx \\
&= \sum_n |C_n|^2,
\end{aligned}$$

where we used the fact that $\phi_n(x)$ are a set of **orthonormal** eigenfunctions. That is, the integral

$$\int_{-\infty}^{\infty} \phi_m^*(x)\phi_n(x)dx$$

is equal to 0 if $m \neq n$ and is equal to 1 if $m = n$. Normalization of $\psi(x)$ is equivalent to demanding

$$\sum_n |C_n|^2 = 1.$$

In this sum, each term $|C_n|^2$ gives the **probability of finding the particle in the energy eiegenstate** $\phi_n(x)$. On the measurement of the energy, since the particle has to be in one of the energy eigenstates, the sum of the probabilities $|C_n|^2$ must add up to 1, giving us $\sum_n |C_n|^2 = 1$.

If the wave function of a particle has the expansion

$$\psi(x) = \sum_n C_n \phi_n(x)$$

in terms of the energy eigenfunctions, then, on the measurement of its energy, the probability of obtaining its energy to be E_m is $|C_m|^2$. If we have a very large number of such particles in identical potential wells, the simultaneous measurement of energies of these particles will give a **distribution of energies**, E_1 with probability $|C_1|^2$, E_2 with probability $|C_2|^2$ and so on. The average value of energy is $\sum_n E_n |C_n|^2$, which is precisely the expectation value of the Hamiltonian

$$\int_{-\infty}^{\infty} \psi^*(x) \hat{H} \psi(x) dx.$$

I urge you to calculate this expectation value for yourself and verify that you get the sum mentioned above.

This argument can be extended to other operators also. It can be shown that, any **Hermitian operator has a set of orthonormal eigenfunctions with real eigenvalues**. Consider such an operator $\hat{\mathcal{A}}$. We solve its eigenfunction equation

$$\hat{\mathcal{A}} f_n(x) = a_n f_n(x),$$

to obtain the eigenfunctions $f_n(x)$ and the corresponding eigenvalues a_n. Given a wave function $\psi(x)$, we can expand it as a linear combination

$$\psi(x) = \sum_n D_n f_n(x),$$

where D_n are constants. As in the previous case, we can show that a measurement of the physical quantity corresponding to $\hat{\mathcal{A}}$ yields one of a_n as a the measured value and the probability of obtaining this value is $|D_n|^2$. And the expectation value of the observable corresponding to $\hat{\mathcal{A}}$ is $\sum_n a_n |D_n|^2$.