# Quantum Mechanics in Medicine

Presented by

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## 3.7 Probability Conservation and the Hermiticity of the Hamiltonian

If the operator $\hat{A}$ satisfy the condition $\boxed{\int \Psi^* \hat{A}\Psi \, d\mathbf{r} = \int (\hat{A}\Psi)^* \Psi \, d\mathbf{r}}$

is called Hermitian operator.

We shall now show that the conservation of probability implies that the Hamiltonian operator **H** appearing in the Schrödinger equation is **Hermitian**.

In terms of **H**, the Schrödinger equation can be written as

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi \qquad \ldots(3.30)$$

The complex conjugate of this equation is

$$-i\hbar \frac{\partial \Psi^*}{\partial t} = (H\Psi)^* \qquad \ldots(3.31)$$

Using these equations, we can write

$$\frac{\partial}{\partial t}\int \Psi^* \Psi d\mathbf{r} = \int \left( \Psi^* \frac{\partial \Psi}{\partial t} + \Psi \frac{\partial \Psi^*}{\partial t} \right) d\mathbf{r} \qquad \ldots(3.32)$$

$$= (i\hbar)^{-1} \int [\Psi^*(H\Psi) - \Psi(H\Psi)^*] d\mathbf{r}$$

Since the left-hand side is zero, we obtain

$$\boxed{\int \Psi^*(H\Psi) d\mathbf{r} = \int (H\Psi)^* \Psi \, d\mathbf{r}} \qquad \ldots(3.33)$$

Operators which satisfy this condition are called Hermitian. Thus, *H* is an Hermitian operator.

## 3.8 Probability Current Density

From equation (3.28)

$$\frac{\partial}{\partial t}\int_V P(\mathbf{r}, t) \, d\mathbf{r} = -\int_V \nabla \cdot \mathbf{j} \, d\mathbf{r}$$

and since this equation is true for any arbitrary volume, we have

$$\boxed{\frac{\partial}{\partial t} P(\mathbf{r}, t) + \nabla \cdot \mathbf{j}(\mathbf{r}, t) = 0} \qquad \ldots(3.34)$$

This is called the equation of continuity.

The vector $\boldsymbol{j}(\boldsymbol{r},t)$ is called the probability current density.

If $\nabla\cdot\boldsymbol{j}=0$ , then for that state the probability density is constant in time. Such states are called stationary states.

## 3.8 Expectation Values of Dynamical Variables

- In quantum mechanics a particle is represented by a wave function which can be obtained by solving the Schrödinger equation and contains all the available information about the particle.
- The dynamical variables of the particle (position, momentum, ….) can be extracted from the wave function Ψ.
- Since Ψ has a probabilistic interpretation, so that exact information about the variables cannot be obtained.
- We obtain only the expectation value of a quantity, which is the average of a large number of measurements on the same system.
- The expectation value of a physical quantity is always real.

*To find the position expectation value* $\langle r\rangle$*:*

Since $P(\mathbf{r},t)=\Psi^*(\mathbf{r},t)\,\Psi(\mathbf{r},t)$ is interpreted as the position probability density at the point $\mathbf{r}$ at the time $t$, the *expectation value* of the position vector $\mathbf{r}$ is given by

$$\langle\mathbf{r}\rangle=\int\mathbf{r}\,P(\mathbf{r},t)d\mathbf{r} \qquad \ldots(3.35)$$

$$=\int\Psi^*(\mathbf{r},t)\,\mathbf{r}\,\Psi(\mathbf{r},t)d\mathbf{r} \qquad \ldots(3.36)$$

where $\Psi(\mathbf{r},t)$ is normalized. This equation is equivalent to the three equations

$$\langle x\rangle = \int \Psi^* \, x \, \Psi \, d\mathbf{r}$$

$$\langle y\rangle = \int \Psi^* \, y \, \Psi \, d\mathbf{r} \qquad \ldots(3.37)$$

$$\langle z\rangle = \int \Psi^* \, z \, \Psi \, d\mathbf{r}$$

- The expectation value is a function only of the time because the space coordinates have been integrated out.
- The expectation value of a physical quantity is always real.

*The expectation value of any quantity which is a function of* ***r*** *and t* would be;

$$\boxed{\langle f(\mathbf{r},t)\rangle = \int \Psi^*(\mathbf{r},t)\, f(\mathbf{r},t)\, \Psi(\mathbf{r},t)\, d\mathbf{r}} \qquad \ldots(3.38)$$

As an example, the expectation value of the potential energy is

$$\langle V(\mathbf{r},t)\rangle = \int \Psi^*(\mathbf{r},t)\, V(\mathbf{r},t)\, \Psi(\mathbf{r},t)\, d\mathbf{r} \qquad \ldots(3.39)$$

The expectation values for quantities which are functions of momentum or of both position and momentum by using the ***operator representations***

$$\hat{\mathbf{p}} = -i\hbar\, \boldsymbol{\nabla}$$

$$p^2 = -\hbar^2\, \nabla^2$$

$$\hat{E} = i\hbar\frac{\partial}{\partial t}$$

**Q: How these differential operators are to be combined with the position probability density $\Psi^*\,\Psi$ to obtain the total energy expressions?**

**Answer:** by using the classical expression for the total energy

$$E = \frac{p^2}{2m} + V$$

And the expectation values;

$$\langle E\rangle = \left\langle \frac{p^2}{2m}\right\rangle + \langle V\rangle \qquad \ldots(3.40)$$

Replacing $E$ and $p^2$ by the corresponding operators, we get

$$\left\langle i\hbar\frac{\partial}{\partial t}\right\rangle = \left\langle -\frac{\hbar^2}{2m}\nabla^2\right\rangle + \langle V\rangle \qquad \ldots(3.41)$$

This equation must be consistent with the Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2\nabla^2}{2m}\Psi + V\Psi$$

Multiplying by $\Psi^*$ on the left and integrating, we get

$$\int\Psi^*\left(i\hbar\frac{\partial}{\partial t}\right)\Psi\,d\mathbf{r} = \int\Psi^*\left(-\frac{\hbar^2\nabla^2}{2m}\right)\Psi\,d\mathbf{r} + \int\Psi^*V\Psi\,d\mathbf{r} \qquad \ldots(3.42)$$

From (3.40) -(3.42) we have;

$$\langle V\rangle = \int\Psi^*\,\mathrm{V}\,\Psi\,dr \qquad \ldots(3.43)$$

$$\langle E\rangle = \int\Psi^*\,i\hbar\frac{\partial\Psi}{\partial t}\,d\mathbf{r} \qquad \ldots(3.44)$$

$$\langle\mathbf{p}\rangle = \int\Psi^*\,(-i\hbar)\,\boldsymbol{\nabla}\Psi\,d\mathbf{r} \qquad \ldots(3.45)$$

The last equation is equivalent to

$$\left.\begin{aligned}\langle p_x\rangle &= -i\hbar\int\Psi^*\frac{\partial\Psi}{\partial x}\,d\mathbf{r}\\ \langle p_y\rangle &= -i\hbar\int\Psi^*\frac{\partial\Psi}{\partial y}\,d\mathbf{r}\\ \langle p_z\rangle &= -i\hbar\int\Psi^*\frac{\partial\Psi}{\partial z}\,d\mathbf{r}\end{aligned}\right] \qquad \ldots(3.46)$$

**Generalizing the above results:**

$\Psi(\boldsymbol{r},t)$ The normalized wave function which describes the dynamical state of a particle.

$A(\boldsymbol{r},\boldsymbol{p},t)$ the dynamical variable representing a physical quantity associated with the particle.

We calculate the expectation value of $A$ from the expression;

$$\langle A\rangle = \int \Psi^*(\boldsymbol{r},t)\,\hat{A}\,\Psi(\mathbf{r},\mathrm{t})\,\mathrm{d}\mathbf{r}\,, \qquad \text{or}$$

$$\boxed{\langle A\rangle = \int \Psi^*(\mathbf{r},t)\,\hat{A}(\mathbf{r},-i\hbar\nabla,t)\,\Psi(\mathbf{r},t)\,d\mathbf{r}} \qquad \ldots(3.46)$$

Since the *expectation value of a physical quantity is always real*, i.e., $\langle A\rangle^* = \langle A\rangle$

Then the operator $\hat{A}$ must satisfy;

$$\boxed{\int \Psi^*\,\hat{A}\Psi\,d\mathbf{r} = \int (\hat{A}\Psi)^*\,\Psi\,d\mathbf{r}} \qquad \ldots(3.47)$$

Thus, the operator associated with a dynamical quantity must be **Hermitian**.