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Paper: C11T (Quantum Mechanics and Applications)
Topic: Schrodinger Equation

In the previous E-learning materials, we have discussed the significance of wave function and its use in the calculations of expectation values of dynamical variables. Here in this material, we will learn to calculate the wave function itself.

Time-independent Schrödinger Equation:

We have already discussed what a wave function is and the physical significance of it. Now we will discuss how to get the wave function $\Psi(x,t)$ in the place. The answer is to solve the Schrodinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi = i\hbar\frac{\partial\Psi}{\partial t} \qquad \text{—— (1)}$$

given a specific potential $V(x,t)$. But for the time-being we will only consider potential without time-dependence i.e. $V(x)$. So, if the potential V is independent of time then we can solve the Schrödinger equation by the method of separation of variables. In this method we consider the solutions of the following form:

$$\Psi(x,t) = \psi(x)\,\phi(t) \qquad \text{—— (2)}$$

where $\psi(x)$ is a function x only and $\phi(t)$ is a function of t only. Though these separable solutions are only a small subset of all the solutions, we will see in the end that these separable solutions can be put together to form the most general solutions of the Schrödinger equation.

From eqn. (2), we get

$$\frac{\partial \Psi}{\partial t} = \psi \frac{d\phi}{dt} \qquad \text{——— (3)}$$

and
$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2 \psi}{dx^2} \phi \qquad \text{——— (4)}$$

Now, using eqn. (3) and eqn. (4) we get from eqn. (1)

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} \phi + V \psi \phi = i\hbar \psi \frac{d\phi}{dt}$$

or,
$$-\frac{\hbar^2}{2m} \frac{1}{\psi} \frac{d^2\psi}{dx^2} + V = i\hbar \frac{1}{\phi} \frac{d\phi}{dt} \qquad \text{—— (5)}$$

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Now, left hand side of eqn. (5) is a function of x-only and right hand side is a function of t-only. This is possible ~~not~~ only when both sides are equal to some constant. Let us consider this constant as E. So, we can write

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V = E$$

$$\text{or, } \boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi} \quad \text{——— (6)}$$

and $\quad i\hbar \frac{1}{\phi}\frac{d\phi}{dt} = E$

$$\text{or, } \frac{d\phi}{dt} = -i\frac{E}{\hbar}\phi \quad \text{——— (7)}$$

The solution of equation (7) is easy to get and is given by $\phi = C e^{-\frac{iEt}{\hbar}}$. But we can avoid the constant factor C here and can include it in ψ as our ~~solu~~ full solution is the product $\psi(x)\phi(t)$.

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So we write

$$\phi(t) = e^{-\frac{iEt}{\hbar}} \quad \text{——— (8)}$$

The equation (6) is quite analogous to the Schrödinger equation, but it is independent of time. So, this eqn. (6) is called the time-independent Schrödinger equation. We can not solve this equation until the potential $V(x)$ is given.

We will solve the time-independent Schrödinger equation for some specific potentials in the next few study materials. But here will now discuss some important features of the separable solutions $\psi(x)\phi(t)$.

(i) <u>Separable solutions are Stationary States.</u>

Though the wave function $\Psi(x,t) = \psi(x)\, e^{-\frac{iEt}{\hbar}}$ — (9) is time dependent, but the probability of finding the particle at position x and time t does not depend on time as

$$|\Psi(x,t)|^2 = \Psi(x,t)^* \Psi(x,t)$$

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$$= \psi^* e^{\frac{iEt}{\hbar}} \psi e^{-\frac{iEt}{\hbar}}$$

$$= \psi^* \psi = |\psi(x)|^2 \quad \text{——} (10)$$

Also we can now show that expectation value of any dynamical variable ~~is~~ does not depend on time. Using eqn. (9), we can rewrite the formulae for expectation value as

$$\langle Q(x,p) \rangle = \int \psi^* Q\left(x, -i\hbar \frac{d}{dx}\right) \psi \, dx \quad \text{——} (11)$$

So, $\langle Q(x,p) \rangle$ is constant in time. Hence, the expectation value for position $\langle x \rangle$ is constant which means the expectation value for momentum

$$\langle p \rangle = m \frac{d}{dt} \langle x \rangle = 0 \quad .$$

This is why the separable solutions are called the stationary states.

(ii) <u>Separable solutions are states of definite total energy.</u>

The sum of the kinetic energy and potential energy is called the Hamiltonian i.e.

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$$H(x,p) = \frac{p^2}{2m} + V(x) \quad \text{——} (12)$$

In the operator form,

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \quad \text{——} (13)$$

Now, the time-independent Schrödinger eqn. (6) can be written as

$$\hat{H}\psi = E\psi \quad \text{——} (14)$$

This equation is called energy eigen value equation. Expectation value of the Hamiltonian can now be calculated as

$$\langle H\rangle = \int \psi^* \hat{H}\psi\, dx$$

$$= E\int \psi^*\psi\, dx \quad [\text{Using eqn. } (14)]$$

$$\text{or, } \langle H\rangle = E\int |\psi(x)|^2\, dx$$

$$= E \quad \text{——} (15)$$

~~As~~ as $\int |\psi(x)|^2 dx$ is the total probability which is 1. Now,

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$$\hat{H}^2\psi = \hat{H}(\hat{H}\psi) = \hat{H}(E\psi)$$
$$= E\hat{H}\psi$$
$$= E^2\psi \quad \text{——— (16)}$$

Therefore the standard deviation in the measurement of the total energy is given by

$$\sigma_H = \sqrt{\langle H^2\rangle - \langle H\rangle^2}$$
$$= \sqrt{E^2 - E^2}$$
$$= 0 \quad \text{——— (17)}$$

$$\langle H^2\rangle = \int \psi^* H^2 \psi \, dx$$
$$= E^2 \int \psi^* \psi \, dx$$
$$= E^2$$

Zero standard deviation means that every measurements results into same value of total energy E. So, every separable solutions corresponds to a definite total energy.

(iii) General solution to the Schrödinger equation is a linear combination of the separable solutions.

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We will see in our future discussions that the time independent Schrödinger equation has infinite number of solutions $\psi_1(x)$, $\psi_2(x)$, $\psi_3(x)$, ...; each of them corresponding to different total energy E_1, E_2, E_3, ... So, we can write

$$\Psi_1(x,t) = \psi_1(x)\, e^{-\frac{iE_1 t}{\hbar}}$$

$$\Psi_2(x,t) = \psi_2(x)\, e^{-\frac{iE_2 t}{\hbar}}$$

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$$\Psi_n(x,t) = \psi_n(x)\, e^{-\frac{iE_n t}{\hbar}} \quad \text{——— (18)}$$

Schrödinger equation (eqn.(1)) has the property that any linear combination of ~~the~~ solutions is also a solution. So, the general solution can be written as

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \Psi_n(x,t) \quad \text{——— (19)}$$

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or, $$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-\frac{iE_n t}{\hbar}} \quad \text{——} (20)$$

Every solution to the Schrödinger eqn. (eqn. (1)) can actually be written in the above form (eqn. (20)) by ~~choo~~ finding correct co-efficients $c_1, c_2, c_3, \ldots$.

Reference:

1. *Introduction to Quantum Mechanics - David J. Griffiths*