Lecture 2

The Wave Function

Study Goal of This Lecture

- Time-independent Schrödinger Equation.
- Requirements of wavefunctions.

2.1 Time-Independent Schrödinger Equation

Last lecture we discussed the consequences of the wave-particle duality and finally reach the point to introduce the time-independent Schrödinger equation(T.I.S.E.):

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\psi(\vec{r}). \tag{2.1}$$

All stationary states of a particle under the influence of potential $V(\vec{r})$ must satisfy this equation.

Q: Why the stationary state of a particle must satisfy the T.I.S.E. ?

2.1.1 Hamiltonian operator

Note that we can further identify on the left hand side of the Schrödinger equation:

$$\underbrace{\{-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\}}_{\substack{\text{something acting}\\ \text{on the wavefunction}}}\psi(\vec{r}) = \overbrace{E}^{\substack{\text{energy,}\\ \text{a real number}}}\psi(\vec{r}), \tag{2.2}$$

we can define an “operator” called “Hamiltonian”

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}). \tag{2.3}$$

e.g. for $\frac{d}{dx}$, $\frac{d}{dx}(x^2) = 2x$

***operator**: acting on a function to generate a different function.*

***operand**: the subject of an operator.*

Here $\hat{H}$ is an operator that is related to the total energy of the system. With $\hat{H}$, we can rewrite the Schrödinger equation as:

$$\hat{H}\psi(\vec{r}) = E\psi(\vec{r}). \tag{2.4}$$

This is a different yet equivalent way to write the time-independent Schrödinger equation. $\psi(\vec{r})$ that satisfies $\hat{H}\psi(\vec{r}) = E\psi(\vec{r})$ is a stationary wave function. Normally, one can find infinite-number of wave functions(states) that satisfy the T.I.S.E.

Notice that solving Schrödinger equation is to find wave functions that when “operated” by $\hat{H}$, yield the same functions with a real proportional constant. This kind of equation posts an “eigenvalue problem”.

When $\hat{H}\psi(\vec{r}) = E\psi(\vec{r})$, we say $\psi(\vec{r})$ is an eigenfunction of $\hat{H}$ and E is the eigenvalue. Solving time-independent Schrödinger equation is to find the eigenfunctions of the Hamiltonian operator $\hat{H}$.

$$\hat{H}\psi_n(\vec{r}) = E_n\psi_n(\vec{r}). \tag{2.5}$$

In Equ (2.5), $\psi_n(\vec{r})$ is the eigenfunction of $\hat{H}$ and E_n is the eigenvalue associate with $\psi_n(\vec{r})$. We normally can find infinite number of solutions. Such eigenvalue problems are not at all difficult to understand.

- eigenfunction of $\frac{d}{dx}$?
- eigenfunction of $\frac{d^2}{dx^2}$?
- ......

observable $\leftrightarrow$ operator

energy $\leftrightarrow$ $\hat{H}$

Quantum mechanics concern many operators. Actually each classical physical observable corresponds to a quantum operator.

Operators are central in quantum mechanics, actually, each physically measurable quantity has an operator associated with it, for example: we have identified the operator for energy $\Rightarrow$ Hamiltonian.

$$\hat{H} \longleftrightarrow -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}).$$

Note

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}^2}{2m} + \hat{V},$$

therefore we can identify

$$\hat{H} \longleftrightarrow V(\vec{r})\cdot \quad \text{[multiply by } V(\vec{r})\text{]},$$

$$\hat{p}_x \longleftrightarrow -i\hbar\frac{\partial}{\partial x},$$

$$\hat{r} \longleftrightarrow \vec{r}\cdot \quad \text{[multiply by } V(\vec{r})\text{]}.$$

From here we can construct operators for any observables in quantum mechanics. We will elaborate this point in the next class when we discuss about operators.

2.1.2 Correspondence Principle

The "correspondence principle" provides a standard procedure to write down a quantum operator from the definition of its classical counterpart.

1. Find expresion for the observable in terms of p and x. e.g. $\vec{l} = \vec{r} \times \vec{p}$
2. Replace $\vec{r} \leftrightarrow \hat{r}$, $\vec{p} \leftrightarrow \hat{p}$. e.g. $\hat{L} = \hat{r} \times \hat{p}$

2.2 Requirements of Wavefunctions

2.2.1 Max Born's interpretation

The key subject in Schrödinger equation is ψ: the wave function. Max Born pointed out that ψ does not have any physical meanung, and it is just a mathematical object that allows us to calculate experimentally measurable quantities. On the other hand, the absolute square of ψ has a physical interpretation:

The probability of finding the particle in an infinitesimal volume ($d\tau = dxdydz$) at $\vec{r}$ is given by $\psi^*(\vec{r})\psi(\vec{r})d\tau \equiv |\psi(\vec{r})|^2 d\tau$.
Thus, $|\psi(\vec{r})|^2$ is the probability density of finding the particle at $\vec{r}$.
(Note the dimension of $\psi(x)$ is $L^{-\frac{1}{2}}$ in 1-D and $L^{-\frac{3}{2}}$ in 3-D.)

Thinking: probability of finding someone in this class who is "exactly" 20 years old $\leftarrow$ What do we normally mean by age $=$ 20? A range!

Note that

$$|\psi(x)|^2 : \text{probability density}$$

$$|\psi(x)|^2 dx : \text{probability of finding the particle between } x \text{ and } x + dx$$

It is important to seperate probability density from probability.

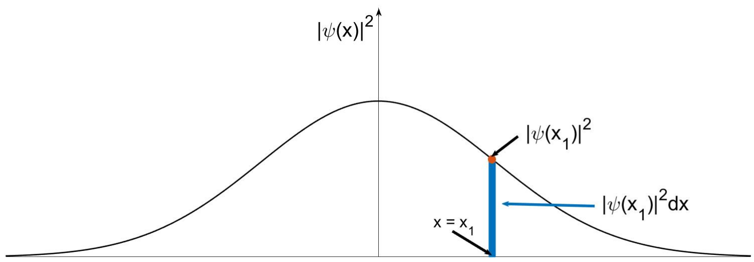

Figure 2.1: Probability density

In order to fulfill this probability interpretation, a physical admissible wavefunction should satisfy the following conditions:

1. continuous everywhere in space. (i.e. finite $\hat{p}$)

2. finite at any position.

3. single-valued for all $\vec{r}$

4. $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$ (1-D)

   $\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\psi(\vec{r})|^2 d\tau = 1$ (3-D)

   normalization condition.

5. $\lim_{x\to\pm\infty} \psi(x) = 0$

These conditions will be used to solve T.I.S.E..

Also, for two wavefunctions, ψ_i and ψ_j,

$$\text{if} \int \psi_i^* \psi_j d\tau = 0 \Rightarrow \text{orthogonal.} \tag{2.6}$$

$$\text{if} \int \psi_i^* \psi_j d\tau = \delta_{ij} \Rightarrow \text{orthornormal.} \tag{2.7}$$

$$\delta_{ij} = \begin{cases} 0 & \text{for } i \neq j \\ 1 & \text{for } i = j \end{cases}, \quad \text{Kronecker delta.} \tag{2.8}$$

$\int_{-\infty}^{\infty} \psi_1 \psi_2 \, dx$ $\equiv$ inner product, more contents would show up in Lecture 3.