PHY 301

Quantum Mechanics

Chongfeng Ling

2021-2022

Contents

1 Introduction

Quantum: quantities can vary by discrete amounts.

Mechanics: study of motion.

1.1 Franklin's Oil-Drop Experiment

Spilled a spoonful (2 ml) of oil on the surface of a lake and extended to about 2000 m^2, but not more. This experiment shows the **existent** and **size** of atoms.

$$V = Sh$$

$$h = \frac{V}{S} \sim \frac{2 \times 10^{-6}}{2 \times 10^{3}} \text{ m} \sim 10^{-9} \text{ m}$$

Atomic and molecular scales are **nanometric**

1.2 From Classical Mechanics to Quantum Mechanics

In classical mechanics, position is a function of time. **Deterministic**.

In quantum mechanics, the position of a particle is a random variable. **Probabilistic**.

2 Wave Function

2.1 Definition in 1-D space

Definition 2.1 (Wave Function)**.** *For a small particle living in a **one-dimensional space**, the wave function* Ψ *is a complex-valued function of space and time:*

$$\Psi : \mathbf{R} \times \mathbf{R} \to \mathbb{C}$$

$$(x, t) \mapsto \Psi(x, t) \in \mathbf{C}$$

Remark 2.1. $|\Psi(x,t)|^2$ *is the p.d.f. of finding the particle in position* x *at time* t*.*

Remark 2.2. $\int_a^b |\Psi(x,t)|^2 dx$ *is the c.d.f of finding the particle between position* $[a, b]$ *at time* t*.*

Remark 2.3. *Integration is over **space**,* t *is a **parameter**.*

2.2 Mean and variance of the position

These two statistics are expressed as integrals over the entire space. They are **deterministic functions of time**. Given wave function Ψ, then we have:

$$\langle x\rangle(t) = \int_{-\infty}^{+\infty} x|\Psi(x,t)|^2 dx$$

$$\langle Var(x)\rangle(t) = \int_{-\infty}^{+\infty} (x - \langle x\rangle(t))^2 |\Psi(x,t)|^2 dx$$

$$[\Psi] = \frac{1}{\sqrt{L}}$$

2.3 Example: probability density of position for classical object

...

3 The Schrödinger equation

One dimension's Schrödinger equation for wave wave function Ψ ($x \in \mathbf{R}$ is a space coordinate, t is time, V is a **real-valued potential**) is

$$\boxed{i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t)} \tag{1}$$

Complex conjugate form is

$$\boxed{-i\hbar\frac{\partial\Psi^*}{\partial t}(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi^*(x,t) + V(x)\Psi^*(x,t)} \tag{2}$$

Planck constant $\hbar$ is

$$\hbar = \frac{h}{2\pi} \simeq 1.05 \times 10^{-34}\ \mathrm{kg}\cdot\mathrm{m}^2\cdot\mathrm{s}^{-1}$$

Assumption 3.1. *Ψ and all its derivatives are smooth and go to zero when $|x|$ goes to infinity, faster than any negative power of x.*

3.1 Normalization

Due to its definition, the wave function has to be normalized at all time. That is, for all t, we have

$$\boxed{\int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x,t)dx = 1} \tag{3}$$

Remark 3.1. *Not all solutions of the Schrödinger equation are wave function.*

$\boxed{\textit{parameter } A?}$

Theorem 3.1. *A normalized wave function stays normalized.*

Proof. For a normalized wave function at time $t = 0$:

$$\int_{-\infty}^{\infty} \Psi^*(x,0)\Psi(x,0)dx = 1$$

consider $t > 0$:

$$
\begin{aligned}
&\frac{d}{dt}\left(\int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x,t)dx\right) \\
&= \int_{-\infty}^{+\infty} \frac{\partial \Psi^*(x,t)}{\partial t}\Psi(x,t)dx + \int_{-\infty}^{+\infty} \Psi^*(x,t)\frac{\partial \Psi(x,t)}{\partial t}dx \\
&= \frac{1}{i\hbar}\int_{-\infty}^{+\infty}\left(+\frac{\hbar^2}{2m}\frac{\partial^2\Psi^*(x,t)}{\partial x^2} - V(x)\Psi^*(x,t)\right)\Psi(x,t)dx+ \\
&\frac{1}{i\hbar}\int_{-\infty}^{+\infty}\Psi^*(x,t)\left(-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t)\right)dx \\
&= \frac{\hbar}{2mi}\left(\left[\Psi\frac{\partial}{\partial x}\Psi^*\right]_{-\infty}^{+\infty} - \int\frac{\partial}{\partial x}\Psi^*\frac{\partial}{\partial x}\Psi dx\right. \\
&\left. - \left[\Psi^*\frac{\partial}{\partial x}\Psi\right]_{-\infty}^{+\infty} + \int\frac{\partial}{\partial x}\Psi\frac{\partial}{\partial x}\Psi^* dx\right) \\
&= 0
\end{aligned}
$$

by Assumption 3.1. Hence, Ψ is normalized at all time. □

3.2 Linear momentum

We can not know actual position of a particle, hence we use the expectation of position $\langle x\rangle(t)$ instead.

$$\boxed{\langle x\rangle(t) = \int_{-\infty}^{+\infty}\Psi^*(x,t)x\Psi(x,t)dx} \tag{4}$$

the velocity of a particle is

$$\boxed{\langle V\rangle = \frac{d\langle x\rangle}{dt}} \tag{5}$$

the average linear momentum is

$$\boxed{\langle p\rangle = \int_{-\infty}^{+\infty}\Psi^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi(x,t)dx} \tag{6}$$

Proof. ... □

3.3 From the Schrödinger equation to the Newton law

Ehrenfest's theorem

$$\frac{d\langle p\rangle}{dt} = -\left\langle V'(x)\right\rangle \tag{7}$$

$\boxed{\textit{obey classical laws?}}$

3.4 Correspondence principle

$\boxed{\textit{why use operator?}}$

$\boxed{\hbar \textit{ to } 0?}$

Energy = kinetic energy + potential energy

Position operator ...

Linear-momentum operator ...

Hamiltonian operator ...

3.5 Separable solutions: time-independent solutions

Consider one kind of solutions of Schrödinger equation in the form:

$$\Psi(x,t) =: \psi(x)\phi(t)$$

the Schrödinger equation becomes:

$$i\hbar\psi(x)\phi'(t) = -\frac{\hbar^2}{2m}\psi''(x)\phi(t) + V(x)\psi(x)\phi(t) \tag{8}$$

$$i\hbar\frac{\phi'(t)}{\phi(t)} = -\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} + V(x) \tag{9}$$

Eq.9 is satisfied for all values of the independent variables x and t, hence there exists a **constant number** E that Eq.9 $= E$ for both sides. We have

$$i\hbar\frac{\phi'(t)}{\phi(t)} = E \tag{10}$$

$$-\frac{\hbar^2}{2m}\frac{\psi''(x)}{\psi(x)} + V(x) = E \tag{11}$$

Time-dependent factor Eq.10 ...

Space-dependent factor Eq.11 ...

Remark 3.2. *E is a constant number.*

Remark 3.3. *E is a real number.*

Proof. ... □

Remark 3.4. $E \geq min(V(x))$

Proof. ... □

3.6 Example: the infinite square well

...

3.7 The free particle: time-dependent solutions

...