Lecture 2

Wednesday, September 13, 2023 15:54

The time-independent Schrödinger equation

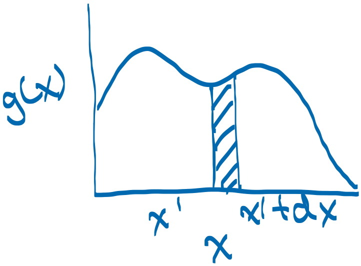
$$-\underbrace{\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}}_{\text{kinetic energy}}+\underbrace{V(x)\psi(x)}_{\text{potential energy}}=E\psi(x)$$

Probability

$$\lim_{N\to\infty}\frac{M}{N}$$

probability that event A occurs when performing an experiment N times, where in M of these events, A occurs

continuous: consider the probability that a particle will be found between x and $x+dx$



g(x) : probability density

$|\psi|^2$: probability density in QM

$$\int_a^b |\psi|^2 dx = \Pr(a \le x \le b)$$

$\uparrow$ probability

$$\boxed{\int_{-\infty}^{\infty} |\psi|^2 dx = 1}$$

i.e. the particle is somewhere on the x-axis

normalized

Complex Numbers

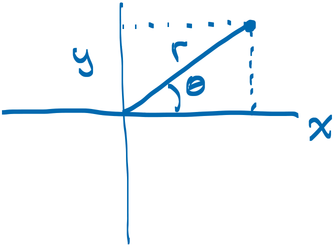
complex number z is a number of the form

$z = x + iy$, where $i \equiv \sqrt{-1}$

where x and y are real

if $x=0$, $y\neq 0$: pure imaginary number

$x = \mathrm{Re}(z)$, $y = \mathrm{Im}(z)$



graphical representation in the complex plane

r : absolute value or modulus of z; denoted $|z|$

$$|z| = r = (x^2+y^2)^{\frac{1}{2}} \qquad \tan\theta = \frac{y}{x}$$

$$x = r\cos\theta, \quad y = r\sin\theta$$

$$z = x + iy$$

$$z = r\cos\theta + ir\sin\theta$$

using Euler's formula

$$e^{i\theta} = \cos\theta + i\sin\theta$$

$z = re^{i\theta}$ (θ is in radians)

complex conjugate z^*

$z^* \equiv x - iy = re^{-i\theta}$

z is real if and only if $z = z^*$

$(z^*)^* = z$

$$zz^* = (x+iy)(x-iy)$$

$$= x^2 + \cancel{ixy} - \cancel{ixy} - \overset{-1}{i^2}\, y^2$$

$$= x^2 + y^2 = r^2$$

$$zz^* = |z|^2$$

$z_1 = r_1 e^{i\theta_1}$, $z_2 = r_2 e^{i\theta_2}$

$z_1 z_2 = r_1 r_2 e^{i(\theta_1+\theta_2)}$ product

$\dfrac{z_1}{z_2} = \dfrac{r_1}{r_2} e^{i(\theta_1-\theta_2)}$ quotient

$|\psi^2| = |\psi|^2 = \psi^* \psi$ where ψ is a complex wavefunction

Differential Equations

- ordinary differential equations; i.e. only one independent variable

3rd order

$$y''' + 2x(y')^2 + y^2 \sin x = 3e^x$$

nth derivatives of y raised to mth power

order: order of the highest derivative in the equation

$$A_n(x)y^{(n)} + A_{n-1}(x)y^{(n-1)} + \dots$$

$$+ A_1(x)y' + A_0(x)y = g(x)$$

linear differential equation

- A's and g are functions of x only

– y and its derivatives appear to the first power

if $g(x) = 0$: homogeneous ; otherwise inhomogeneous

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V(x)\Psi(x) = E\Psi(x)$$

- homogeneous
- linear
- ordinary
- second order

$$\boxed{1}\, y'' + P(x)\,y' + Q(x)\,y = 0$$

dividing by coefficient of y'', every linear homogeneous second-order differential equation can be written in this form

$$\boxed{y = c_1 y_1 + c_2 y_2}$$

general solution

y_1 and y_2 are linearly independent

$$c_1 y_1'' + c_2 y_2'' + P(x) c_1 y_1' + P(x) c_2 y_2'$$

$$+ Q(x) c_1 y_1 + Q(x) c_2 y_2$$

$$= c_1 \underline{\left[y_1'' + P(x) y_1' + Q(x) y_1 \right]}$$

$$+ c_2 \underline{\left[y_2'' + P(x) y_2' + Q(x) y_2 \right]}$$

$$= c_1 (0) + c_2 (0) = 0$$

Special case: constant coefficients

$$y'' + p y' + q y = 0 \qquad (2.6)$$

tentatively assume a solution of the form

$y = e^{ax}$ substitute into (2.6)

$$a^2 e^{ax} + ape^{ax} + q e^{ax} = 0$$

$$\boxed{a^2 + pa + q = 0}$$ auxiliary equation

quadratic ; two roots a_1 and a_2

if $a_1 \neq a_2$: two independent solutions

$$\boxed{y = c_1 e^{a_1 x} + c_2 e^{a_2 x}}$$

$$y'' + 6y' - 7y = 0$$

write auxiliary equation

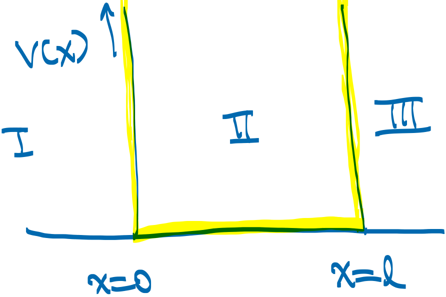
$a^2 + 6a - 7 = 0$ $\quad a_1 = 1$, $a_2 = -7$

general solution :

$$y = c_1 e^{x} + c_2 e^{-7x}$$

Particle in a one-dimensional box

to ∞ to ∞



$V(x) = 0$ from $x = 0$ to $x = \ell$

$V(x) = \infty$ elsewhere

In regions I and III, the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} \overset{\curvearrowright}{+\infty\psi} = E\psi$$

negligible ↙

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (E-\infty)\psi$$

divide by $-\frac{\hbar^2}{2m}$

$$\frac{d^2\psi}{dx^2} = \infty\psi$$

$$\psi = \frac{1}{\infty}\frac{d^2\psi}{dx^2}$$

therefore $\psi = 0$ outside of the box

$$\psi_{I} = 0, \quad \psi_{III} = 0$$

For region II, $V(x) = 0$, so we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} + 0\,\psi_{II} = E\psi_{II}$$

divide by $-\frac{\hbar^2}{2m}$

$$\frac{d^2\psi_{II}}{dx^2} = -\frac{2mE}{\hbar^2}\psi_{II}$$

$$\frac{d^2\psi_{II}}{dx^2} + \frac{2m}{\hbar^2}E\psi_{II} = 0$$

m : mass of the particle

$$a^2 + 2mE\hbar^{-2} = 0$$

auxiliary equation

$$a^2 = -2mE\hbar^{-2}$$

$$a = \pm\sqrt{\frac{-2mE}{\hbar^2}}$$

$$a = \pm\frac{(2mE)^{\frac{1}{2}}}{\hbar}\, i$$

solution to ψ_{II} :

$$\psi_{II} = c_1 e^{i(2mE)^{\frac{1}{2}}/\hbar \cdot x} + c_2 e^{-i(2mE)^{\frac{1}{2}}/\hbar \cdot x}$$

let $\theta \equiv \frac{(2mE)^{\frac{1}{2}}}{\hbar}\, x$

$$\psi_{II} = c_1 e^{i\theta} + c_2 e^{-i\theta}$$

recall $e^{i\theta} = \cos\theta + i\sin\theta$

$e^{-i\theta} = \cos\theta - i\sin\theta$

$$\psi_{II} = c_1\cos\theta + i c_1\sin\theta + c_2\cos\theta - i c_2\sin\theta$$

$$= (c_1 + c_2)\cos\theta + (ic_1 - ic_2)\sin\theta$$

$$\boxed{\psi_{II} = A\cos\theta + B\sin\theta}$$